# International Tables for Crystallography

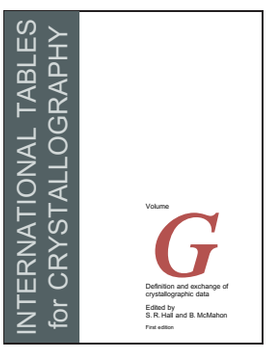
## Volume G: Definition and exchange of crystallographic data

Edited by S. R. Hall and B. McMahon

### Chapter 4.5. Macromolecular dictionary (mmCIF)

(P. M. D. Fitzgerald, J. D. Westbrook, P. E. Bourne, B. McMahon, K. D. Watenpaugh and H. M. Berman)






Volume G describes the standard data exchange and archival file format (CIF) used throughout crystallography. It provides in-depth information vital for small-molecule, inorganic and macromolecular crystallographers, mineralogists, chemists, materials scientists, solid-state physicists and others who wish to record or use the results of a single-crystal or powder diffraction experiment. The volume also provides the detailed data ontology necessary for programmers and database managers to design interoperable computer applications. The accompanying CD-ROM contains the CIF dictionaries in machine-readable form and a collection of libraries and utility programs.

This volume is an essential guide and reference for programmers of crystallographic software, data managers handling crystal-structure information and practising crystallographers who need to use CIF.

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# 4.5. Macromolecular dictionary (mmCIF)

BY P. M. D. FITZGERALD, J. D. WESTBROOK, P. E. BOURNE, B. MCMAHON, K. D. WATENPAUGH AND H. M. BERMAN

This is version 2.0.09 of the macromolecular CIF dictionary (mmCIF). The philosophy behind this dictionary and the history of its development are described in Chapter 1.1. A detailed commentary on the use of the dictionary is given in Chapter 3.6.

**Category groups**

| | |
|---|---|
| atom_group | Categories that describe the properties of atoms. |
| audit_group | Categories that describe dictionary maintenance and identification. |
| cell_group | Categories that describe the unit cell. |
| chemical_group | Categories that describe chemical properties and nomenclature. |
| chem_comp_group | Categories that describe components of chemical structure. |
| chem_link_group | Categories that describe links between components of chemical structure. |
| citation_group | Categories that provide bibliographic references. |
| computing_group | Categories that describe the computational details of the experiment. |
| compliance_group | Categories that are included in this dictionary specifically to comply with previous dictionaries. |
| database_group | Categories that hold references to entries in databases that contain related information. |
| diffrn_group | Categories that describe details of the diffraction experiment. |
| entity_group | Categories that describe chemical entities. |
| entry_group | Categories that pertain to the entire data block. |
| exptl_group | Categories that hold details of the experimental conditions. |
| geom_group | Categories that hold details of molecular and crystal geometry. |
| iucr_group | Categories that are used for manuscript submission and internal processing by the staff of the International Union of Crystallography. |
| pdb_group | Categories that pertain to the file-format or data-processing codes used by the Protein Data Bank. |
| phasing_group | Categories that describe phasing. |
| refine_group | Categories that describe refinement. |
| refln_group | Categories that describe the details of reflection measurements. |
| struct_group | Categories that contain details about the crystallographic structure. |
| symmetry_group | Categories that describe symmetry information. |

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**ATOM_SITE**

Data items in the ATOM_SITE category record details about the atom sites in a macromolecular crystal structure, such as the positional coordinates, atomic displacement parameters, magnetic moments and directions. The data items for describing anisotropic atomic displacement factors are only used if the corresponding items are not given in the ATOM_SITE_ANISOTROP category.

Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_site.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_site.group_PDB
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_comp_id
_atom_site.label_asym_id
_atom_site.label_seq_id
_atom_site.label_alt_id
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.occupancy
_atom_site.B_iso_or_equiv
_atom_site.footnote_id
_atom_site.auth_seq_id
_atom_site.id
ATOM N  N   VAL  A  11  .  25.369  30.691  11.795  1.00
     17.93  .  11   1
ATOM C  CA  VAL  A  11  .  25.970  31.965  12.332  1.00
     17.75  .  11   2
ATOM C  C   VAL  A  11  .  25.569  32.010  13.808  1.00
     17.83  .  11   3
ATOM O  O   VAL  A  11  .  24.735  31.190  14.167  1.00
     17.53  .  11   4
ATOM C  CB  VAL  A  11  .  25.379  33.146  11.540  1.00
     17.66  .  11   5
ATOM C  CG1 VAL  A  11  .  25.584  33.034  10.030  1.00
     18.86  .  11   6
ATOM C  CG2 VAL  A  11  .  23.933  33.309  11.872  1.00
     17.12  .  11   7
ATOM N  N   THR  A  12  .  26.095  32.930  14.590  1.00
     18.97  4  12   8
ATOM C  CA  THR  A  12  .  25.734  32.995  16.032  1.00
     19.80  4  12   9
ATOM C  C   THR  A  12  .  24.695  34.106  16.113  1.00
     20.92  4  12  10
ATOM O  O   THR  A  12  .  24.869  35.118  15.421  1.00
     21.84  4  12  11
ATOM C  CB  THR  A  12  .  26.911  33.346  17.018  1.00
     20.51  4  12  12
ATOM O  OG1 THR  A  12  3  27.946  33.921  16.183  0.50
     20.29  4  12  13
```

```
ATOM O  OG1 THR  A  12  4  27.769  32.142  17.103  0.50
     20.59  4  12  14
ATOM C  CG2 THR  A  12  3  27.418  32.181  17.878  0.50
     20.47  4  12  15
ATOM C  CG2 THR  A  12  4  26.489  33.778  18.426  0.50
     20.00  4  12  16
ATOM N  N   ILE  A  13  .  23.664  33.855  16.884  1.00
     22.08  .  13  17
ATOM C  CA  ILE  A  13  .  22.623  34.850  17.093  1.00
     23.44  .  13  18
ATOM C  C   ILE  A  13  .  22.657  35.113  18.610  1.00
     25.77  .  13  19
ATOM O  O   ILE  A  13  .  23.123  34.250  19.406  1.00
     26.28  .  13  20
ATOM C  CB  ILE  A  13  .  21.236  34.463  16.492  1.00
     22.67  .  13  21
ATOM C  CG1 ILE  A  13  .  20.478  33.469  17.371  1.00
     22.14  .  13  22
ATOM C  CG2 ILE  A  13  .  21.357  33.986  15.016  1.00
     21.75  .  13  23
# - - - - data truncated for brevity - - - -
HETATM C C1 APS  C   .  1   4.171  29.012   7.116  0.58
     17.27  1 300  101
HETATM C C2 APS  C   .  1   4.949  27.758   6.793  0.58
     16.95  1 300  102
HETATM O O3 APS  C   .  1   4.800  26.678   7.393  0.58
     16.85  1 300  103
HETATM N N4 APS  C   .  1   5.930  27.841   5.869  0.58
     16.43  1 300  104
# - - - - data truncated for brevity - - - -
```

**_atom_site.adp_type** (*code*)

***_atom_site_adp_type*** (*cif_core.dic 2.3*)

A standard code used to describe the type of atomic displacement parameters used for the site.

Related item: **_atom_site.thermal_displace_type** (alternate).

The data value must be one of the following:

| | |
|---|---|
| Uani | anisotropic $U^{ij}$ |
| Uiso | isotropic $U$ |
| Uovl | overall $U$ |
| Umpe | multipole expansion $U$ |
| Bani | anisotropic $B^{ij}$ |
| Biso | isotropic $B$ |
| Bovl | overall $B$ |

**[atom_site]**

**_atom_site.aniso_B[1][1]** (*float, su*)

The [1][1] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site.aniso_B[1][1]_esd** (associated esd), **_atom_site.aniso_U[1][1]** (conversion constant), **_atom_site_anisotrop.U[1][1]** (conversion constant), **_atom_site.aniso_U[1][1]** (alternate exclusive), **_atom_site_anisotrop.B[1][1]** (alternate exclusive), **_atom_site_anisotrop.U[1][1]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_B[1][1]_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_B[1][1].**

Related items: **_atom_site.aniso_B[1][1]** (associated value), **_atom_site.aniso_U[1][1]_esd** (conversion constant), **_atom_site_anisotrop.U[1][1]_esd** (conversion constant), **_atom_site.aniso_U[1][1]_esd** (alternate exclusive), **_atom_site_anisotrop.B[1][1]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][1]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_B[1][2]** (*float, su*)

The [1][2] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site.aniso_B[1][2]_esd** (associated esd), **_atom_site.aniso_U[1][2]** (conversion constant), **_atom_site_anisotrop.U[1][2]** (conversion constant), **_atom_site.aniso_U[1][2]** (alternate exclusive), **_atom_site_anisotrop.B[1][2]** (alternate exclusive), **_atom_site_anisotrop.U[1][2]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_B[1][2]_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_B[1][2].**

Related items: **_atom_site.aniso_B[1][2]** (associated value), **_atom_site.aniso_U[1][2]_esd** (conversion constant), **_atom_site_anisotrop.U[1][2]_esd** (conversion constant), **_atom_site.aniso_U[1][2]_esd** (alternate exclusive), **_atom_site_anisotrop.B[1][2]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][2]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_B[1][3]** (*float, su*)

The [1][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on

Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: `_atom_site.aniso_B[1][3]_esd` (associated esd), `_atom_site.aniso_U[1][3]` (conversion constant), `_atom_site_anisotrop.U[1][3]` (conversion constant), `_atom_site.aniso_U[1][3]` (alternate exclusive), `_atom_site_anisotrop.B[1][3]` (alternate exclusive), `_atom_site_anisotrop.U[1][3]` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[1][3]_esd`** (*float*)
The standard uncertainty (estimated standard deviation) of `_atom_site.aniso_B[1][3]`.

Related items: `_atom_site.aniso_B[1][3]` (associated value), `_atom_site.aniso_U[1][3]_esd` (conversion constant), `_atom_site_anisotrop.U[1][3]_esd` (conversion constant), `_atom_site.aniso_U[1][3]_esd` (alternate exclusive), `_atom_site_anisotrop.B[1][3]_esd` (alternate exclusive), `_atom_site_anisotrop.U[1][3]_esd` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[2][2]`** (*float, su*)
The [2][2] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: `_atom_site.aniso_B[2][2]_esd` (associated esd), `_atom_site.aniso_U[2][2]` (conversion constant), `_atom_site_anisotrop.U[2][2]` (conversion constant), `_atom_site.aniso_U[2][2]` (alternate exclusive), `_atom_site_anisotrop.B[2][2]` (alternate exclusive), `_atom_site_anisotrop.U[2][2]` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[2][2]_esd`** (*float*)
The standard uncertainty (estimated standard deviation) of `_atom_site.aniso_B[2][2]`.

Related items: `_atom_site.aniso_B[2][2]` (associated value), `_atom_site.aniso_U[2][2]_esd` (conversion constant), `_atom_site_anisotrop.U[2][2]_esd` (conversion constant), `_atom_site.aniso_U[2][2]_esd` (alternate exclusive), `_atom_site_anisotrop.B[2][2]_esd` (alternate exclusive), `_atom_site_anisotrop.U[2][2]_esd` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[2][3]`** (*float, su*)
The [2][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: `_atom_site.aniso_B[2][3]_esd` (associated esd), `_atom_site.aniso_U[2][3]` (conversion constant), `_atom_site_anisotrop.U[2][3]` (conversion constant), `_atom_site.aniso_U[2][3]` (alternate exclusive), `_atom_site_anisotrop.B[2][3]` (alternate exclusive), `_atom_site_anisotrop.U[2][3]` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[2][3]_esd`** (*float*)
The standard uncertainty (estimated standard deviation) of `_atom_site.aniso_B[2][3]`.

Related items: `_atom_site.aniso_B[2][3]` (associated value), `_atom_site.aniso_U[2][3]_esd` (conversion constant), `_atom_site_anisotrop.U[2][3]_esd` (conversion constant), `_atom_site.aniso_U[2][3]_esd` (alternate exclusive), `_atom_site_anisotrop.B[2][3]_esd` (alternate exclusive), `_atom_site_anisotrop.U[2][3]_esd` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[3][3]`** (*float, su*)
The [3][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: `_atom_site.aniso_B[3][3]_esd` (associated esd), `_atom_site.aniso_U[3][3]` (conversion constant), `_atom_site_anisotrop.U[3][3]` (conversion constant), `_atom_site.aniso_U[3][3]` (alternate exclusive), `_atom_site_anisotrop.B[3][3]` (alternate exclusive), `_atom_site_anisotrop.U[3][3]` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_B[3][3]_esd`** (*float*)
The standard uncertainty (estimated standard deviation) of `_atom_site.aniso_B[3][3]`.

Related items: `_atom_site.aniso_B[3][3]` (associated value), `_atom_site.aniso_U[3][3]_esd` (conversion constant), `_atom_site_anisotrop.U[3][3]_esd` (conversion constant), `_atom_site.aniso_U[3][3]_esd` (alternate exclusive), `_atom_site_anisotrop.B[3][3]_esd` (alternate exclusive), `_atom_site_anisotrop.U[3][3]_esd` (alternate exclusive). `[atom_site]`

**`_atom_site.aniso_ratio`** (*float*)
Ratio of the maximum to minimum principal axes of displacement (thermal) ellipsoids.

The permitted range is $[1.0, \infty)$.

Related item: `_atom_site_anisotrop.ratio` (alternate exclusive). `[atom_site]`

**_atom_site.aniso_U[1][1]** (*float, su*)
The [1][1] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[1][1]_esd** (associated esd), **_atom_site.aniso_B[1][1]** (conversion constant), **_atom_site_anisotrop.B[1][1]** (conversion constant), **_atom_site.aniso_B[1][1]** (alternate exclusive), **_atom_site_anisotrop.B[1][1]** (alternate exclusive), **_atom_site_anisotrop.U[1][1]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[1][3]** (*float, su*)
The [1][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[1][3]_esd** (associated esd), **_atom_site.aniso_B[1][3]** (conversion constant), **_atom_site_anisotrop.B[1][3]** (conversion constant), **_atom_site.aniso_B[1][3]** (alternate exclusive), **_atom_site_anisotrop.B[1][3]** (alternate exclusive), **_atom_site_anisotrop.U[1][3]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[1][1]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[1][1].**

Related items: **_atom_site.aniso_U[1][1]** (associated value), **_atom_site.aniso_B[1][1]_esd** (conversion constant), **_atom_site_anisotrop.B[1][1]_esd** (conversion constant), **_atom_site.aniso_B[1][1]_esd** (alternate exclusive), **_atom_site_anisotrop.B[1][1]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][1]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[1][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[1][3].**

Related items: **_atom_site.aniso_U[1][3]** (associated value), **_atom_site.aniso_B[1][3]_esd** (conversion constant), **_atom_site_anisotrop.B[1][3]_esd** (conversion constant), **_atom_site.aniso_B[1][3]_esd** (alternate exclusive), **_atom_site_anisotrop.B[1][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][3]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[1][2]** (*float, su*)
The [1][2] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[1][2]_esd** (associated esd), **_atom_site.aniso_B[1][2]** (conversion constant), **_atom_site_anisotrop.B[1][2]** (conversion constant), **_atom_site.aniso_B[1][2]** (alternate exclusive), **_atom_site_anisotrop.B[1][2]** (alternate exclusive), **_atom_site_anisotrop.U[1][2]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[2][2]** (*float, su*)
The [2][2] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[2][2]_esd** (associated esd), **_atom_site.aniso_B[2][2]** (conversion constant), **_atom_site_anisotrop.B[2][2]** (conversion constant), **_atom_site.aniso_B[2][2]** (alternate exclusive), **_atom_site_anisotrop.B[2][2]** (alternate exclusive), **_atom_site_anisotrop.U[2][2]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[1][2]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[1][2].**

Related items: **_atom_site.aniso_U[1][2]** (associated value), **_atom_site.aniso_B[1][2]_esd** (conversion constant), **_atom_site_anisotrop.B[1][2]_esd** (conversion constant), **_atom_site.aniso_B[1][2]_esd** (alternate exclusive), **_atom_site_anisotrop.B[1][2]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][2]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[2][2]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[2][2].**

Related items: **_atom_site.aniso_U[2][2]** (associated value), **_atom_site.aniso_B[2][2]_esd** (conversion constant), **_atom_site_anisotrop.B[2][2]_esd** (conversion constant), **_atom_site.aniso_B[2][2]_esd** (alternate exclusive), **_atom_site_anisotrop.B[2][2]_esd** (alternate exclusive), **_atom_site_anisotrop.U[2][2]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[2][3]** (*float, su*)
The [2][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[2][3]_esd** (associated esd), **_atom_site.aniso_B[2][3]** (conversion constant), **_atom_site_anisotrop.B[2][3]** (conversion constant), **_atom_site.aniso_B[2][3]** (alternate exclusive), **_atom_site_anisotrop.B[2][3]** (alternate exclusive), **_atom_site_anisotrop.U[2][3]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[2][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[2][3].**

Related items: **_atom_site.aniso_U[2][3]** (associated value), **_atom_site.aniso_B[2][3]_esd** (conversion constant), **_atom_site_anisotrop.B[2][3]_esd** (conversion constant), **_atom_site.aniso_B[2][3]_esd** (alternate exclusive), **_atom_site_anisotrop.B[2][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[2][3]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[3][3]** (*float, su*)
The [3][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site.aniso_U[3][3]_esd** (associated esd), **_atom_site.aniso_B[3][3]** (conversion constant), **_atom_site_anisotrop.B[3][3]** (conversion constant), **_atom_site.aniso_B[3][3]** (alternate exclusive), **_atom_site_anisotrop.B[3][3]** (alternate exclusive), **_atom_site_anisotrop.U[3][3]** (alternate exclusive). **[atom_site]**

**_atom_site.aniso_U[3][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.aniso_U[3][3].**

Related items: **_atom_site.aniso_U[3][3]** (associated value), **_atom_site.aniso_B[3][3]_esd** (conversion constant), **_atom_site_anisotrop.B[3][3]_esd** (conversion constant), **_atom_site.aniso_B[3][3]_esd** (alternate exclusive), **_atom_site_anisotrop.B[3][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[3][3]_esd** (alternate exclusive). **[atom_site]**

**_atom_site.attached_hydrogens** (*int*)
***_atom_site_attached_hydrogens*** (*cif_core.dic 2.0.1*)
The number of hydrogen atoms attached to the atom at this site excluding any hydrogen atoms for which coordinates (measured or calculated) are given.

The permitted range is [0, 8].

Examples: '2' (water oxygen), '1' (hydroxyl oxygen), '4' (ammonium nitrogen).

**[atom_site]**

***_atom_site.auth_asym_id** (*code*)
An alternative identifier for **_atom_site.label_asym_id** that may be provided by an author in order to match the identification used in the publication that describes the structure.

*The following item(s) have an equivalent role in their respective categories:*

***_geom_angle.atom_site_auth_asym_id_1***, ***_geom_angle.atom_site_auth_asym_id_2***, ***_geom_angle.atom_site_auth_asym_id_3***, ***_geom_bond.atom_site_auth_asym_id_1***, ***_geom_bond.atom_site_auth_asym_id_2***, ***_geom_contact.atom_site_auth_asym_id_1***, ***_geom_contact.atom_site_auth_asym_id_2***, ***_geom_hbond.atom_site_auth_asym_id_A***, ***_geom_hbond.atom_site_auth_asym_id_D***, ***_geom_hbond.atom_site_auth_asym_id_H***, ***_geom_torsion.atom_site_auth_asym_id_1***, ***_geom_torsion.atom_site_auth_asym_id_2***, ***_geom_torsion.atom_site_auth_asym_id_3***, ***_geom_torsion.atom_site_auth_asym_id_4***, ***_struct_conf.beg_auth_asym_id***, ***_struct_conf.end_auth_asym_id***, ***_struct_conn.ptnr1_auth_asym_id***, ***_struct_conn.ptnr2_auth_asym_id***, ***_struct_mon_nucl.auth_asym_id***, ***_struct_mon_prot.auth_asym_id***, ***_struct_mon_prot_cis.auth_asym_id***, ***_struct_ncs_dom_lim.beg_auth_asym_id***, ***_struct_ncs_dom_lim.end_auth_asym_id***, ***_struct_sheet_range.beg_auth_asym_id***, ***_struct_sheet_range.end_auth_asym_id***, ***_struct_site_gen.auth_asym_id***. **[atom_site]**

**_atom_site.auth_atom_id** (*atcode*)
An alternative identifier for **_atom_site.label_atom_id** that may be provided by an author in order to match the identification used in the publication that describes the structure.

*The following item(s) have an equivalent role in their respective categories:*

***_geom_angle.atom_site_auth_atom_id_1***, ***_geom_angle.atom_site_auth_atom_id_2***, ***_geom_angle.atom_site_auth_atom_id_3***, ***_geom_bond.atom_site_auth_atom_id_1***, ***_geom_bond.atom_site_auth_atom_id_2***, ***_geom_contact.atom_site_auth_atom_id_1***, ***_geom_contact.atom_site_auth_atom_id_2***, ***_geom_hbond.atom_site_auth_atom_id_A***, ***_geom_hbond.atom_site_auth_atom_id_D***, ***_geom_hbond.atom_site_auth_atom_id_H***, ***_geom_torsion.atom_site_auth_atom_id_1***, ***_geom_torsion.atom_site_auth_atom_id_2***, ***_geom_torsion.atom_site_auth_atom_id_3***, ***_geom_torsion.atom_site_auth_atom_id_4***, ***_struct_conn.ptnr1_auth_atom_id***, ***_struct_conn.ptnr2_auth_atom_id***, ***_struct_sheet_hbond.range_1_beg_auth_atom_id***, ***_struct_sheet_hbond.range_1_end_auth_atom_id***, ***_struct_sheet_hbond.range_2_beg_auth_atom_id***, ***_struct_sheet_hbond.range_2_end_auth_atom_id***, ***_struct_site_gen.auth_atom_id***. **[atom_site]**

### _atom_site.auth_comp_id (*code*)

An alternative identifier for _atom_site.label_comp_id that may be provided by an author in order to match the identification used in the publication that describes the structure.

*The following item(s) have an equivalent role in their respective categories:*

_geom_angle.atom_site_auth_comp_id_1,
_geom_angle.atom_site_auth_comp_id_2,
_geom_angle.atom_site_auth_comp_id_3,
_geom_bond.atom_site_auth_comp_id_1,
_geom_bond.atom_site_auth_comp_id_2,
_geom_contact.atom_site_auth_comp_id_1,
_geom_contact.atom_site_auth_comp_id_2,
_geom_hbond.atom_site_auth_comp_id_A,
_geom_hbond.atom_site_auth_comp_id_D,
_geom_hbond.atom_site_auth_comp_id_H,
_geom_torsion.atom_site_auth_comp_id_1,
_geom_torsion.atom_site_auth_comp_id_2,
_geom_torsion.atom_site_auth_comp_id_3,
_geom_torsion.atom_site_auth_comp_id_4,
_struct_conf.beg_auth_comp_id,
_struct_conf.end_auth_comp_id,
_struct_conn.ptnr1_auth_comp_id,
_struct_conn.ptnr2_auth_comp_id,
_struct_mon_nucl.auth_comp_id,
_struct_mon_prot.auth_comp_id,
_struct_mon_prot_cis.auth_comp_id,
_struct_ncs_dom_lim.beg_auth_comp_id,
_struct_ncs_dom_lim.end_auth_comp_id,
_struct_sheet_range.beg_auth_comp_id,
_struct_sheet_range.end_auth_comp_id,
_struct_site_gen.auth_comp_id. [atom_site]

### _atom_site.auth_seq_id (*code*)

An alternative identifier for _atom_site.label_seq_id that may be provided by an author in order to match the identification used in the publication that describes the structure. Note that this is not necessarily a number, that the values do not have to be positive, and that the value does not have to correspond to the value of _atom_site.label_seq_id. The value of _atom_site.label_seq_id is required to be a sequential list of positive integers. The author may assign values to _atom_site.auth_seq_id in any desired way. For instance, the values may be used to relate this structure to a numbering scheme in a homologous structure, including sequence gaps or insertion codes. Alternatively, a scheme may be used for a truncated polymer that maintains the numbering scheme of the full length polymer. In all cases, the scheme used here must match the scheme used in the publication that describes the structure.

*The following item(s) have an equivalent role in their respective categories:*

_geom_angle.atom_site_auth_seq_id_1,
_geom_angle.atom_site_auth_seq_id_2,
_geom_angle.atom_site_auth_seq_id_3,
_geom_bond.atom_site_auth_seq_id_1,
_geom_bond.atom_site_auth_seq_id_2,
_geom_contact.atom_site_auth_seq_id_1,
_geom_contact.atom_site_auth_seq_id_2,
_geom_hbond.atom_site_auth_seq_id_A,
_geom_hbond.atom_site_auth_seq_id_D,
_geom_hbond.atom_site_auth_seq_id_H,
_geom_torsion.atom_site_auth_seq_id_1,
_geom_torsion.atom_site_auth_seq_id_2,
_geom_torsion.atom_site_auth_seq_id_3,
_geom_torsion.atom_site_auth_seq_id_4,
_struct_conf.beg_auth_seq_id,
_struct_conf.end_auth_seq_id,
_struct_conn.ptnr1_auth_seq_id,
_struct_conn.ptnr2_auth_seq_id,
_struct_mon_nucl.auth_seq_id,
_struct_mon_prot.auth_seq_id,
_struct_mon_prot_cis.auth_seq_id,
_struct_ncs_dom_lim.beg_auth_seq_id,
_struct_ncs_dom_lim.end_auth_seq_id,
_struct_sheet_hbond.range_1_beg_auth_seq_id,
_struct_sheet_hbond.range_1_end_auth_seq_id,
_struct_sheet_hbond.range_2_beg_auth_seq_id,
_struct_sheet_hbond.range_2_end_auth_seq_id,
_struct_sheet_range.beg_auth_seq_id,
_struct_sheet_range.end_auth_seq_id,
_struct_site_gen.auth_seq_id. [atom_site]

### _atom_site.B_equiv_geom_mean (*float, su*)

_atom_site_B_equiv_geom_mean (*cif_core.dic 2.0.1*)

Equivalent isotropic atomic displacement parameter, $B_{\rm eq}$, in ångströms squared, calculated as the geometric mean of the anisotropic atomic displacement parameters.

$$B_{\rm eq} = (B_i B_j B_k)^{1/3},$$

where $B_n$ = the principal components of the orthogonalized $B^{ij}$.

The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

The permitted range is $[0.0, \infty)$.

Related items: _atom_site.B_equiv_geom_mean_esd (associated esd), _atom_site.U_equiv_geom_mean (conversion constant). [atom_site]

### _atom_site.B_equiv_geom_mean_esd (*float*)

The standard uncertainty (estimated standard deviation) of _atom_site.B_equiv_geom_mean.

Related items: _atom_site.B_equiv_geom_mean (associated value), _atom_site.U_equiv_geom_mean (conversion constant). [atom_site]

### _atom_site.B_iso_or_equiv (*float, su*)

_atom_site_B_iso_or_equiv (*cif_core.dic 2.0.1*)

Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $B_{\rm eq}$, calculated from the anisotropic displacement parameters.

$$B_{\rm eq} = (1/3) \sum_i \left[ \sum_j (B^{ij} A_i A_j a_i^* a_j^*) \right],$$

where $A$ = the real-space cell lengths and $a^*$ = the reciprocal-space cell lengths; $B^{ij} = 8\pi^2 U^{ij}$.

Reference: Fischer, R. X. & Tillmanns, E. (1988). *Acta Cryst.* C**44**, 775–776.

The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: _atom_site.B_iso_or_equiv_esd (associated esd), _atom_site.U_iso_or_equiv (conversion constant). [atom_site]

### _atom_site.B_iso_or_equiv_esd (*float*)

The standard uncertainty (estimated standard deviation) of _atom_site.B_iso_or_equiv.

Related items: _atom_site.B_iso_or_equiv (associated value), _atom_site.U_iso_or_equiv_esd (conversion constant). [atom_site]

### _atom_site.calc_attached_atom (*code*)

_atom_site_calc_attached_atom (*cif_core.dic 2.0.1*)

The _atom_site.id of the atom site to which the 'geometry-calculated' atom site is attached.

[atom_site]

**_atom_site.calc_flag** (*ucode*)
***_atom_site_calc_flag*** (*cif_core.dic 2.0.1*)
A standard code to signal whether the site coordinates have been determined from the intensities or calculated from the geometry of surrounding sites, or have been assigned dummy values. The abbreviation 'c' may be used in place of 'calc'.
The data value must be one of the following:

| | |
|---|---|
| d | determined from experimental measurements |
| calc | calculated from molecular geometry |
| c | abbreviation for 'calc' |
| dum | dummy site with meaningless coordinates |

**[atom_site]**

**_atom_site.Cartn_x** (*float, su*)
***_atom_site_Cartn_x*** (*cif_core.dic 2.0.1*)
The *x* atom-site coordinate in ångströms specified according to a set of orthogonal Cartesian axes related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_atom_site.Cartn_x_esd** (associated esd). **[atom_site]**

**_atom_site.Cartn_x_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.Cartn_x**.
Related item: **_atom_site.Cartn_x** (associated value). **[atom_site]**

**_atom_site.Cartn_y** (*float, su*)
***_atom_site_Cartn_y*** (*cif_core.dic 2.0.1*)
The *y* atom-site coordinate in ångströms specified according to a set of orthogonal Cartesian axes related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_atom_site.Cartn_y_esd** (associated esd). **[atom_site]**

**_atom_site.Cartn_y_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.Cartn_y**.
Related item: **_atom_site.Cartn_y** (associated value). **[atom_site]**

**_atom_site.Cartn_z** (*float, su*)
***_atom_site_Cartn_z*** (*cif_core.dic 2.0.1*)
The *z* atom-site coordinate in ångströms specified according to a set of orthogonal Cartesian axes related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_atom_site.Cartn_z_esd** (associated esd). **[atom_site]**

**_atom_site.Cartn_z_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.Cartn_z**.
Related item: **_atom_site.Cartn_z** (associated value). **[atom_site]**

**_atom_site.chemical_conn_number**
***_atom_site_chemical_conn_number*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_chemical_conn_atom.number** in the CHEMICAL_CONN_ATOM category.

**_atom_site.constraints** (*line*)
***_atom_site_constraints*** (*cif_core.dic 2.0.1*)
A description of the constraints applied to parameters at this site during refinement. See also **_atom_site.refinement_flags** and **_refine.ls_number_constraints**.
Example: 'pop=1.0-pop(Zn3)'. **[atom_site]**

**_atom_site.details** (*text*)
***_atom_site_description*** (*cif_core.dic 2.0.1*)
A description of special aspects of this site. See also **_atom_site.refinement_flags**.
Example: 'Ag/Si disordered'. **[atom_site]**

**_atom_site.disorder_assembly** (*code*)
***_atom_site_disorder_assembly*** (*cif_core.dic 2.0.1*)
A code which identifies a cluster of atoms that show long-range positional disorder but are locally ordered. Within each such cluster of atoms, **_atom_site.disorder_group** is used to identify the sites that are simultaneously occupied. This field is only needed if there is more than one cluster of disordered atoms showing independent local order.
*Note:* This data item would not in general be used in a macromolecular data block.

**[atom_site]**

**_atom_site.disorder_group** (*code*)
***_atom_site_disorder_group*** (*cif_core.dic 2.0.1*)
A code which identifies a group of positionally disordered atom sites that are locally simultaneously occupied. Atoms that are positionally disordered over two or more sites (*e.g.* the hydrogen atoms of a methyl group that exists in two orientations) can be assigned to two or more groups. Sites belonging to the same group are simultaneously occupied, but those belonging to different groups are not. A minus prefix (*e.g.* '-1') is used to indicate sites disordered about a special position.
*Note:* This data item would not in general be used in a macromolecular data block.
Where no value is given, the assumed value is '.'. **[atom_site]**

**_atom_site.footnote_id**
The value of **_atom_site.footnote_id** must match an ID specified by **_atom_sites_footnote.id** in the ATOM_SITES_FOOTNOTE list.

**_atom_site.fract_x** (*float, su*)
***_atom_site_fract_x*** (*cif_core.dic 2.0.1*)
The *x* coordinate of the atom-site position specified as a fraction of **_cell.length_a**.
Related item: **_atom_site.fract_x_esd** (associated esd). **[atom_site]**

**_atom_site.fract_x_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.fract_x**.
Related item: **_atom_site.fract_x** (associated value). **[atom_site]**

**_atom_site.fract_y** (*float, su*)
***_atom_site_fract_y*** (*cif_core.dic 2.0.1*)
The *y* coordinate of the atom-site position specified as a fraction of **_cell.length_b**.
Related item: **_atom_site.fract_y_esd** (associated esd). **[atom_site]**

**_atom_site.fract_y_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.fract_y**.
Related item: **_atom_site.fract_y** (associated value). **[atom_site]**

**_atom_site.fract_z** (*float, su*)
***_atom_site_fract_z*** (*cif_core.dic 2.0.1*)
The *z* coordinate of the atom-site position specified as a fraction of **_cell.length_c**.
Related item: **_atom_site.fract_z_esd** (associated esd). **[atom_site]**

**_atom_site.fract_z_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.fract_z**.
Related item: **_atom_site.fract_z** (associated value). **[atom_site]**

**_atom_site.group_PDB** (*code*)
The group of atoms to which the atom site belongs. This data item is provided for compatibility with the original Protein Data Bank format, and only for that purpose.
The data value must be one of the following:
ATOM
HETATM **[atom_site]**

***_atom_site.id** (*code*)
***_atom_site_label*** (*cif_core.dic 2.0.1*)
The value of **_atom_site.id** must uniquely identify a record in the ATOM_SITE list. Note that this item need not be a number; it can be any unique identifier. This data item was introduced to provide compatibility between small-molecule and macromolecular CIFs. In a small-molecule CIF, **_atom_site_label** is the identifier for the atom. In a macromolecular CIF, the atom identifier is the aggregate of **_atom_site.label_alt_id**, **_atom_site.label_asym_id**, **_atom_site.label_atom_id**, **_atom_site.label_comp_id** and **_atom_site.label_seq_id**. For the two types of files to be compatible, a formal identifier for the category had to be introduced that was independent of the different modes of identifying the atoms. For compatibility with older CIFs, **_atom_site_label** is aliased to **_atom_site.id**.
*The following item(s) have an equivalent role in their respective categories:*
***_atom_site_anisotrop.id***,
***_geom_angle.atom_site_id_1***,
***_geom_angle.atom_site_id_2***,
***_geom_angle.atom_site_id_3***,
***_geom_bond.atom_site_id_1***,
***_geom_bond.atom_site_id_2***,
***_geom_contact.atom_site_id_1***,
***_geom_contact.atom_site_id_2***,
***_geom_hbond.atom_site_id_A***,
***_geom_hbond.atom_site_id_D***,
***_geom_hbond.atom_site_id_H***,
***_geom_torsion.atom_site_id_1***,
***_geom_torsion.atom_site_id_2***,
***_geom_torsion.atom_site_id_3***,
***_geom_torsion.atom_site_id_4***.
Examples: '5', 'C12', 'Ca3g28', 'Fe3+17', 'H*251', 'boron2a', 'C_a_phe_83_a_0', 'Zn_Zn_301_A_0'. **[atom_site]**

***_atom_site.label_alt_id**
A component of the identifier for this atom site. For further details, see the definition of the ATOM_SITE_ALT category. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_atom_site.label_asym_id**
A component of the identifier for this atom site. For further details, see the definition of the STRUCT_ASYM category. This data item is a pointer to **_struct_asym.id** in the STRUCT_ASYM category.

***_atom_site.label_atom_id**
A component of the identifier for this atom site. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_atom_site.label_comp_id**
A component of the identifier for this atom site. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

***_atom_site.label_entity_id**
This data item is a pointer to **_entity.id** in the ENTITY category.

***_atom_site.label_seq_id**
This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

**_atom_site.occupancy** (*float, su*)
***_atom_site_occupancy*** (*cif_core.dic 2.0.1*)
The fraction of the atom type present at this site. The sum of the occupancies of all the atom types at this site may not significantly exceed 1.0 unless it is a dummy site.
Related item: **_atom_site.occupancy_esd** (associated esd). Where no value is given, the assumed value is '1.0'. **[atom_site]**

**_atom_site.occupancy_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.occupancy**.
Related item: **_atom_site.occupancy** (associated value). **[atom_site]**

**_atom_site.refinement_flags** (*code*)
***_atom_site_refinement_flags*** (*cif_core.dic 2.3*)
A concatenated series of single-letter codes which indicate the refinement restraints or constraints applied to this site. This item should not be used. It has been replaced by **_atom_site.refinement_flags_posn**, ***_adp** and ***_occupancy**. It is retained in this dictionary only to provide compatibility with old CIFs.
Related items: **_atom_site.refinement_flags_posn** (replaces), **_atom_site.refinement_flags_adp** (replaces), **_atom_site.refinement_flags_occupancy** (replaces).
The data value must be one of the following:

| | |
|---|---|
| . | no refinement constraints |
| S | special-position constraint on site |
| G | rigid-group refinement of site |
| R | riding-atom site attached to non-riding atom |
| D | distance or angle restraint on site |
| T | thermal displacement constraints |
| U | $U_{iso}$ or $U^{ij}$ restraint (rigid bond) |
| P | partial occupancy constraint |

**[atom_site]**

**_atom_site.refinement_flags_adp** (*code*)
***_atom_site_refinement_flags_adp*** (*cif_core.dic 2.3*)
A code which indicates the refinement restraints or constraints applied to the atomic displacement parameters of this site.
Related item: **_atom_site.refinement_flags_posn** (alternate).
The data value must be one of the following:

| | |
|---|---|
| . | no constraints on atomic displacement parameters |
| T | special-position constraints on atomic displacement parameters |
| U | $U_{iso}$ or $U^{ij}$ restraint (rigid bond) |
| TU | both constraints applied |

**[atom_site]**

**_atom_site.refinement_flags_occupancy** (*code*)
***_atom_site_refinement_flags_occupancy*** (*cif_core.dic 2.3*)
A code which indicates that refinement restraints or constraints were applied to the occupancy of this site.
Related item: **_atom_site.refinement_flags_posn** (alternate).
The data value must be one of the following:

| | |
|---|---|
| . | no constraints on site-occupancy parameters |
| P | site-occupancy constraint |

**[atom_site]**

**_atom_site.refinement_flags_posn** (*code*)
***_atom_site_refinement_flags_posn*** (*cif_core.dic 2.3*)
A code which indicates the refinement restraints or constraints applied to the positional coordinates of this site.
Related item: **_atom_site.refinement_flags_posn** (alternate).
The data value must be one of the following:

| | |
|---|---|
| . | no constraints on positional coordinates |
| D | distance or angle restraint on positional coordinates |
| G | rigid-group refinement of positional coordinates |
| R | riding-atom site attached to non-riding atom |
| S | special-position constraint on positional coordinates |
| DG | combination of the above constraints |
| DR | combination of the above constraints |
| DS | combination of the above constraints |
| GR | combination of the above constraints |
| GS | combination of the above constraints |
| RS | combination of the above constraints |
| DGR | combination of the above constraints |
| DGS | combination of the above constraints |
| DRS | combination of the above constraints |
| GRS | combination of the above constraints |
| DGRS | combination of the above constraints |

**[atom_site]**

**_atom_site.restraints** (*text*)
***_atom_site_restraints*** (*cif_core.dic 2.0.1*)
A description of restraints applied to specific parameters at this site during refinement. See also **_atom_site.refinement_flags** and **_refine.ls_number_restraints**.
Example: 'restrained to planar ring'. **[atom_site]**

**_atom_site.symmetry_multiplicity** (*int*)
***_atom_site_symmetry_multiplicity*** (*cif_core.dic 2.0.1*)
The multiplicity of a site due to the space-group symmetry as is given in *International Tables for Crystallography* Vol. A (2002).
The permitted range is [1, 192]. **[atom_site]**

**_atom_site.thermal_displace_type** (*ucode*)
***_atom_site_thermal_displace_type*** (*cif_core.dic 2.0.1*)
A standard code used to describe the type of atomic displacement parameters used for the site.
The data value must be one of the following:

| | |
|---|---|
| Uani | anisotropic $U^{ij}$ |
| Uiso | isotropic $U$ |
| Uovl | overall $U$ |
| Umpe | multipole expansion $U$ |
| Bani | anisotropic $B^{ij}$ |
| Biso | isotropic $B$ |
| Bovl | overall $B$ |

**[atom_site]**

***_atom_site.type_symbol**
***_atom_site_type_symbol*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_atom_type.symbol** in the ATOM_TYPE category.

**_atom_site.U_equiv_geom_mean** (*float, su*)
***_atom_site_U_equiv_geom_mean*** (*cif_core.dic 2.0.1*)
Equivalent isotropic atomic displacement parameter, $U_{\rm eq}$, in ångströms squared, calculated as the geometric mean of the anisotropic atomic displacement parameters.

$$U_{\rm eq} = (U_i U_j U_k)^{1/3},$$

where $U_n$ = the principal components of the orthogonalized $U^{ij}$.
The permitted range is [0.0, 10.0].
Related items: **_atom_site.U_equiv_geom_mean_esd** (associated esd), **_atom_site.B_equiv_geom_mean** (conversion constant). **[atom_site]**

**_atom_site.U_equiv_geom_mean_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.U_equiv_geom_mean**.
Related items: **_atom_site.U_equiv_geom_mean** (associated value), **_atom_site.B_equiv_geom_mean** (conversion constant). **[atom_site]**

**_atom_site.U_iso_or_equiv** (*float, su*)
***_atom_site_U_iso_or_equiv*** (*cif_core.dic 2.0.1*)
Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, $U_{\rm eq}$, calculated from anisotropic atomic displacement parameters.

$$U_{\rm eq} = (1/3) \sum_i \left[ \sum_j (U^{ij} A_i A_j a_i^* a_j^*) \right],$$

where $A$ = the real-space cell lengths and $a^*$ = the reciprocal-space cell lengths.

Reference: Fischer, R. X. & Tillmanns, E. (1988). *Acta Cryst.* C**44**, 775–776.

The permitted range is [0.0, 10.0].
Related items: **_atom_site.U_iso_or_equiv_esd** (associated esd), **_atom_site.B_iso_or_equiv** (conversion constant). **[atom_site]**

**_atom_site.U_iso_or_equiv_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site.U_iso_or_equiv**.
Related items: **_atom_site.U_iso_or_equiv** (associated value), **_atom_site.B_iso_or_equiv_esd** (conversion constant). **[atom_site]**

**_atom_site.Wyckoff_symbol** (*line*)
***_atom_site_Wyckoff_symbol*** (*cif_core.dic 2.0.1*)
The Wyckoff symbol (letter) as listed in the space-group tables of *International Tables for Crystallography* Vol. A (2002).

**[atom_site]**

## ATOM_SITE_ANISOTROP

Data items in the ATOM_SITE_ANISOTROP category record details about anisotropic displacement parameters. If the ATOM_SITE_ANISOTROP category is used for storing these data, the corresponding ATOM_SITE data items are not used.
Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_site_anisotrop.id**

*Example 1 – based on NDB structure BDL005 of Holbrook, Dickerson & Kim [Acta Cryst. (1985), B**41**, 255–262].*

```
loop_
_atom_site_anisotrop.id
_atom_site_anisotrop.type_symbol
_atom_site_anisotrop.U[1][1]
_atom_site_anisotrop.U[1][2]
_atom_site_anisotrop.U[1][3]
_atom_site_anisotrop.U[2][2]
_atom_site_anisotrop.U[2][3]
_atom_site_anisotrop.U[3][3]
 1  O   8642   4866   7299   -342   -258  -1427
 2  C   5174   4871   6243  -1885  -2051  -1377
 3  C   6202   5020   4395  -1130   -556   -632
 4  O   4224   4700   5046   1105   -161    345
 5  C   8684   4688   4171  -1850   -433   -292
 6  O  11226   5255   3532   -341   2685   1328
 7  C  10214   2428   5614  -2610  -1940    902
 8  C   4590   3488   5827    751   -770    986
 9  N   5014   4434   3447    -17  -1593    539
# ----   abbreviated  ----
```

**_atom_site_anisotrop.B[1][1]** (*float, su*)
***_atom_site_aniso_B_11*** (*cif_core.dic 2.0.1*)
The [1][1] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i \Big[\sum_j (B^{ij}h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[1][1]_esd** (associated esd), **_atom_site.aniso_U[1][1]** (conversion constant), **_atom_site_anisotrop.U[1][1]** (conversion constant), **_atom_site.aniso_B[1][1]** (alternate exclusive), **_atom_site.aniso_U[1][1]** (alternate exclusive), **_atom_site_anisotrop.U[1][1]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[1][1]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[1][1].**

Related items: **_atom_site_anisotrop.B[1][1]** (associated value), **_atom_site.aniso_U[1][1]_esd** (conversion constant), **_atom_site_anisotrop.U[1][1]_esd** (conversion constant), **_atom_site.aniso_B[1][1]_esd** (alternate exclusive), **_atom_site.aniso_U[1][1]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][1]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[1][2]** (*float, su*)
***_atom_site_aniso_B_12*** (*cif_core.dic 2.0.1*)
The [1][2] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i \Big[\sum_j (B^{ij}h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[1][2]_esd** (associated esd), **_atom_site.aniso_U[1][2]** (conversion constant), **_atom_site_anisotrop.U[1][2]** (conversion constant), **_atom_site.aniso_B[1][2]** (alternate exclusive), **_atom_site.aniso_U[1][2]** (alternate exclusive), **_atom_site_anisotrop.U[1][2]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[1][2]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[1][2].**

Related items: **_atom_site_anisotrop.B[1][2]** (associated value), **_atom_site.aniso_U[1][2]_esd** (conversion constant), **_atom_site_anisotrop.U[1][2]_esd** (conversion constant), **_atom_site.aniso_B[1][2]_esd** (alternate exclusive), **_atom_site.aniso_U[1][2]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][2]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[1][3]** (*float, su*)
***_atom_site_aniso_B_13*** (*cif_core.dic 2.0.1*)
The [1][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i \Big[\sum_j (B^{ij}h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[1][3]_esd** (associated esd), **_atom_site.aniso_U[1][3]** (conversion constant), **_atom_site_anisotrop.U[1][3]** (conversion constant), **_atom_site.aniso_B[1][3]** (alternate exclusive), **_atom_site.aniso_U[1][3]** (alternate exclusive), **_atom_site_anisotrop.U[1][3]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[1][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[1][3].**

Related items: **_atom_site_anisotrop.B[1][3]** (associated value), **_atom_site.aniso_U[1][3]_esd** (conversion constant), **_atom_site_anisotrop.U[1][3]_esd** (conversion constant), **_atom_site.aniso_B[1][3]_esd** (alternate exclusive), **_atom_site.aniso_U[1][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[1][3]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[2][2]** (*float, su*)
***_atom_site_aniso_B_22*** (*cif_core.dic 2.0.1*)
The [2][2] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i \Big[\sum_j (B^{ij}h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting

atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[2][2]_esd** (associated esd), **_atom_site.aniso_U[2][2]** (conversion constant), **_atom_site_anisotrop.U[2][2]** (conversion constant), **_atom_site.aniso_B[2][2]** (alternate exclusive), **_atom_site.aniso_U[2][2]** (alternate exclusive), **_atom_site_anisotrop.U[2][2]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[2][2]_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[2][2].**

Related items: **_atom_site_anisotrop.B[2][2]** (associated value), **_atom_site.aniso_U[2][2]_esd** (conversion constant), **_atom_site_anisotrop.U[2][2]_esd** (conversion constant), **_atom_site.aniso_B[2][2]_esd** (alternate exclusive), **_atom_site.aniso_U[2][2]_esd** (alternate exclusive), **_atom_site_anisotrop.U[2][2]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[2][3]** (*float, su*)

***_atom_site_aniso_B_23*** (*cif_core.dic 2.0.1*)

The [2][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[2][3]_esd** (associated esd), **_atom_site.aniso_U[2][3]** (conversion constant), **_atom_site_anisotrop.U[2][3]** (conversion constant), **_atom_site.aniso_B[2][3]** (alternate exclusive), **_atom_site.aniso_U[2][3]** (alternate exclusive), **_atom_site_anisotrop.U[2][3]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[2][3]_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[2][3].**

Related items: **_atom_site_anisotrop.B[2][3]** (associated value), **_atom_site.aniso_U[2][3]_esd** (conversion constant), **_atom_site_anisotrop.U[2][3]_esd** (conversion constant), **_atom_site.aniso_B[2][3]_esd** (alternate exclusive), **_atom_site.aniso_U[2][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[2][3]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[3][3]** (*float, su*)

***_atom_site_aniso_B_33*** (*cif_core.dic 2.0.1*)

The [3][3] element of the anisotropic atomic displacement matrix **B**, which appears in the structure-factor term as

$$T = \exp\Big\{-(1/4)\sum_i\Big[\sum_j(B^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row. The IUCr Commission on Nomenclature recommends against the use of **B** for reporting atomic displacement parameters. **U**, being directly proportional to **B**, is preferred.

Related items: **_atom_site_anisotrop.B[3][3]_esd** (associated esd), **_atom_site.aniso_U[3][3]** (conversion constant), **_atom_site_anisotrop.U[3][3]** (conversion constant), **_atom_site.aniso_B[3][3]** (alternate exclusive), **_atom_site.aniso_U[3][3]** (alternate exclusive), **_atom_site_anisotrop.U[3][3]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.B[3][3]_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.B[3][3].**

Related items: **_atom_site_anisotrop.B[3][3]** (associated value), **_atom_site.aniso_U[3][3]_esd** (conversion constant), **_atom_site_anisotrop.U[3][3]_esd** (conversion constant), **_atom_site.aniso_B[3][3]_esd** (alternate exclusive), **_atom_site.aniso_U[3][3]_esd** (alternate exclusive), **_atom_site_anisotrop.U[3][3]_esd** (alternate exclusive).

**[atom_site_anisotrop]**

***_atom_site_anisotrop.id**

***_atom_site_aniso_label*** (*cif_core.dic 2.0.1*)

This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

**_atom_site_anisotrop.ratio** (*float*)

***_atom_site_aniso_ratio*** (*cif_core.dic 2.0.1*)

Ratio of the maximum to minimum principal axes of displacement (thermal) ellipsoids.

The permitted range is $[1.0, \infty)$.

Related item: **_atom_site.aniso_ratio** (alternate exclusive).

**[atom_site_anisotrop]**

***_atom_site_anisotrop.type_symbol**

***_atom_site_aniso_type_symbol*** (*cif_core.dic 2.0.1*)

This data item is a pointer to **_atom_type.symbol** in the ATOM_TYPE category.

**_atom_site_anisotrop.U[1][1]** (*float, su*)

***_atom_site_aniso_U_11*** (*cif_core.dic 2.0.1*)

The [1][1] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2\sum_i\Big[\sum_j(U^{ij}h_ih_ja_i^*a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either $B$'s or $U$'s, but not as both. The unique elements of the real symmetric matrix are entered by row.

Related items: **_atom_site_anisotrop.U[1][1]_esd** (associated esd), **_atom_site.aniso_B[1][1]** (conversion constant), **_atom_site_anisotrop.B[1][1]** (conversion constant), **_atom_site.aniso_B[1][1]** (alternate exclusive), **_atom_site.aniso_U[1][1]** (alternate exclusive), **_atom_site_anisotrop.B[1][1]** (alternate exclusive).

**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[1][1]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[1][1].**
Related items: **_atom_site_anisotrop.U[1][1]** (associated value),
**_atom_site.aniso_B[1][1]_esd** (conversion constant),
**_atom_site_anisotrop.B[1][1]_esd** (conversion constant),
**_atom_site.aniso_B[1][1]_esd** (alternate exclusive),
**_atom_site.aniso_U[1][1]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[1][1]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[1][2]** (*float, su*)
***_atom_site_aniso_U_12*** (*cif_core.dic 2.0.1*)
The [1][2] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row.
Related items: **_atom_site_anisotrop.U[1][2]_esd** (associated esd),
**_atom_site.aniso_B[1][2]** (conversion constant),
**_atom_site_anisotrop.B[1][2]** (conversion constant),
**_atom_site.aniso_B[1][2]** (alternate exclusive),
**_atom_site.aniso_U[1][2]** (alternate exclusive),
**_atom_site_anisotrop.B[1][2]** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[1][2]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[1][2].**
Related items: **_atom_site_anisotrop.U[1][2]** (associated value),
**_atom_site.aniso_B[1][2]_esd** (conversion constant),
**_atom_site_anisotrop.B[1][2]_esd** (conversion constant),
**_atom_site.aniso_B[1][2]_esd** (alternate exclusive),
**_atom_site.aniso_U[1][2]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[1][2]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[1][3]** (*float, su*)
***_atom_site_aniso_U_13*** (*cif_core.dic 2.0.1*)
The [1][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row.
Related items: **_atom_site_anisotrop.U[1][3]_esd** (associated esd),
**_atom_site.aniso_B[1][3]** (conversion constant),
**_atom_site_anisotrop.B[1][3]** (conversion constant),
**_atom_site.aniso_B[1][3]** (alternate exclusive),
**_atom_site.aniso_U[1][3]** (alternate exclusive),
**_atom_site_anisotrop.B[1][3]** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[1][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[1][3].**
Related items: **_atom_site_anisotrop.U[1][3]** (associated value),
**_atom_site.aniso_B[1][3]_esd** (conversion constant),
**_atom_site_anisotrop.B[1][3]_esd** (conversion constant),
**_atom_site.aniso_B[1][3]_esd** (alternate exclusive),
**_atom_site.aniso_U[1][3]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[1][3]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[2][2]** (*float, su*)
***_atom_site_aniso_U_22*** (*cif_core.dic 2.0.1*)
The [2][2] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row.
Related items: **_atom_site_anisotrop.U[2][2]_esd** (associated esd),
**_atom_site.aniso_B[2][2]** (conversion constant),
**_atom_site_anisotrop.B[2][2]** (conversion constant),
**_atom_site.aniso_B[2][2]** (alternate exclusive),
**_atom_site.aniso_U[2][2]** (alternate exclusive),
**_atom_site_anisotrop.B[2][2]** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[2][2]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[2][2].**
Related items: **_atom_site_anisotrop.U[2][2]** (associated value),
**_atom_site.aniso_B[2][2]_esd** (conversion constant),
**_atom_site_anisotrop.B[2][2]_esd** (conversion constant),
**_atom_site.aniso_B[2][2]_esd** (alternate exclusive),
**_atom_site.aniso_U[2][2]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[2][2]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[2][3]** (*float, su*)
***_atom_site_aniso_U_23*** (*cif_core.dic 2.0.1*)
The [2][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row.
Related items: **_atom_site_anisotrop.U[2][3]_esd** (associated esd),
**_atom_site.aniso_B[2][3]** (conversion constant),
**_atom_site_anisotrop.B[2][3]** (conversion constant),
**_atom_site.aniso_B[2][3]** (alternate exclusive),
**_atom_site.aniso_U[2][3]** (alternate exclusive),
**_atom_site_anisotrop.B[2][3]** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[2][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[2][3].**
Related items: **_atom_site_anisotrop.U[2][3]** (associated value),
**_atom_site.aniso_B[2][3]_esd** (conversion constant),
**_atom_site_anisotrop.B[2][3]_esd** (conversion constant),
**_atom_site.aniso_B[2][3]_esd** (alternate exclusive),
**_atom_site.aniso_U[2][3]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[2][3]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[3][3]** (*float, su*)
***_atom_site_aniso_U_33*** (*cif_core.dic 2.0.1*)
The [3][3] element of the standard anisotropic atomic displacement matrix **U**, which appears in the structure-factor term as

$$T = \exp\Big\{-2\pi^2 \sum_i \Big[\sum_j (U^{ij} h_i h_j a_i^* a_j^*)\Big]\Big\},$$

where $h$ = the Miller indices and $a^*$ = the reciprocal-space cell lengths.

These matrix elements may appear with atomic coordinates in the ATOM_SITE category, or they may appear in the separate ATOM_SITE_ANISOTROP category, but they may not appear in both places. Similarly, anisotropic displacements may appear as either *B*'s or *U*'s, but not as both. The unique elements of the real symmetric matrix are entered by row.
Related items: **_atom_site_anisotrop.U[3][3]_esd** (associated esd),
**_atom_site.aniso_B[3][3]** (conversion constant),
**_atom_site_anisotrop.B[3][3]** (conversion constant),
**_atom_site.aniso_B[3][3]** (alternate exclusive),
**_atom_site.aniso_U[3][3]** (alternate exclusive),
**_atom_site_anisotrop.B[3][3]** (alternate exclusive).
**[atom_site_anisotrop]**

**_atom_site_anisotrop.U[3][3]_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_atom_site_anisotrop.U[3][3].**
Related items: **_atom_site_anisotrop.U[3][3]** (associated value),
**_atom_site.aniso_B[3][3]_esd** (conversion constant),
**_atom_site_anisotrop.B[3][3]_esd** (conversion constant),
**_atom_site.aniso_B[3][3]_esd** (alternate exclusive),
**_atom_site.aniso_U[3][3]_esd** (alternate exclusive),
**_atom_site_anisotrop.B[3][3]_esd** (alternate exclusive).
**[atom_site_anisotrop]**

## ATOM_SITES

Data items in the ATOM_SITES category record details about the crystallographic cell and cell transformations, which are common to all atom sites.
Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_sites.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_atom_sites.entry_id                    '5HVP'
_atom_sites.Cartn_transform_axes
     'c along z, astar along x, b along y'
_atom_sites.Cartn_transf_matrix[1][1] 58.39
_atom_sites.Cartn_transf_matrix[1][2]  0.00
_atom_sites.Cartn_transf_matrix[1][3]  0.00
_atom_sites.Cartn_transf_matrix[2][1]  0.00
_atom_sites.Cartn_transf_matrix[2][2] 86.70
_atom_sites.Cartn_transf_matrix[2][3]  0.00
_atom_sites.Cartn_transf_matrix[3][1]  0.00
_atom_sites.Cartn_transf_matrix[3][2]  0.00
_atom_sites.Cartn_transf_matrix[3][3] 46.27
_atom_sites.Cartn_transf_vector[1]     0.00
_atom_sites.Cartn_transf_vector[2]     0.00
_atom_sites.Cartn_transf_vector[3]     0.00
```

**_atom_sites.Cartn_transf_matrix[1][1]** (*float*)
***_atom_sites_Cartn_tran_matrix_11*** (*cif_core.dic 2.0.1*)
The [1][1] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[1][2]** (*float*)
***_atom_sites_Cartn_tran_matrix_12*** (*cif_core.dic 2.0.1*)
The [1][2] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[1][3]** (*float*)
***_atom_sites_Cartn_tran_matrix_13*** (*cif_core.dic 2.0.1*)
The [1][3] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[2][1]** (*float*)
***_atom_sites_Cartn_tran_matrix_21*** (*cif_core.dic 2.0.1*)
The [2][1] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[2][2]** (*float*)
***_atom_sites_Cartn_tran_matrix_22*** (*cif_core.dic 2.0.1*)
The [2][2] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[2][3]** (*float*)
***_atom_sites_Cartn_tran_matrix_23*** (*cif_core.dic 2.0.1*)
The [2][3] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[3][1]** (*float*)
***_atom_sites_Cartn_tran_matrix_31*** (*cif_core.dic 2.0.1*)
The [3][1] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[3][2]** (*float*)
***_atom_sites_Cartn_tran_matrix_32*** (*cif_core.dic 2.0.1*)
The [3][2] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_matrix[3][3]** (*float*)
***_atom_sites_Cartn_tran_matrix_33*** (*cif_core.dic 2.0.1*)
The [3][3] element of the 3 × 3 matrix used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.Cartn_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_vector[1]** (*float*)
***_atom_sites_Cartn_tran_vector_1*** (*cif_core.dic 2.0.1*)
The [1] element of the three-element vector used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The rotation matrix is defined in **_atom_sites.Cartn_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_vector[2]** (*float*)
***_atom_sites_Cartn_tran_vector_2*** (*cif_core.dic 2.0.1*)
The [2] element of the three-element vector used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The rotation matrix is defined in **_atom_sites.Cartn_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transf_vector[3]** (*float*)
***_atom_sites_Cartn_tran_vector_3*** (*cif_core.dic 2.0.1*)
The [3] element of the three-element vector used to transform fractional coordinates in the ATOM_SITE category to Cartesian coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The rotation matrix is defined in **_atom_sites.Cartn_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{fractional}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.Cartn_transform_axes** (*text*)
***_atom_sites_Cartn_transform_axes*** (*cif_core.dic 2.0.1*)
A description of the relative alignment of the crystal cell axes to the Cartesian orthogonal axes as applied in the transformation matrix **_atom_sites.Cartn_transf_matrix**[][].
Example: 'a parallel to x; b in the plane of y and z'.
**[atom_sites]**

* **_atom_sites.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_atom_sites.fract_transf_matrix[1][1]** (*float*)
*_atom_sites_fract_tran_matrix_11* (*cif_core.dic 2.0.1*)
The [1][1] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[1][2]** (*float*)
*_atom_sites_fract_tran_matrix_12* (*cif_core.dic 2.0.1*)
The [1][2] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[1][3]** (*float*)
*_atom_sites_fract_tran_matrix_13* (*cif_core.dic 2.0.1*)
The [1][3] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[2][1]** (*float*)
*_atom_sites_fract_tran_matrix_21* (*cif_core.dic 2.0.1*)
The [2][1] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[2][2]** (*float*)
*_atom_sites_fract_tran_matrix_22* (*cif_core.dic 2.0.1*)
The [2][2] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[2][3]** (*float*)
*_atom_sites_fract_tran_matrix_23* (*cif_core.dic 2.0.1*)
The [2][3] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[3][1]** (*float*)
*_atom_sites_fract_tran_matrix_31* (*cif_core.dic 2.0.1*)
The [3][1] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[3][2]** (*float*)
*_atom_sites_fract_tran_matrix_32* (*cif_core.dic 2.0.1*)
The [3][2] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_matrix[3][3]** (*float*)
*_atom_sites_fract_tran_matrix_33* (*cif_core.dic 2.0.1*)
The [3][3] element of the 3 × 3 matrix used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 1 translation is defined in **_atom_sites.fract_transf_vector**[].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_vector[1]** (*float*)
***_atom_sites_fract_tran_vector_1*** (*cif_core.dic 2.0.1*)
The [1] element of the three-element vector used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 3 rotation is defined in **_atom_sites.fract_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_vector[2]** (*float*)
***_atom_sites_fract_tran_vector_2*** (*cif_core.dic 2.0.1*)
The [2] element of the three-element vector used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 3 rotation is defined in **_atom_sites.fract_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.fract_transf_vector[3]** (*float*)
***_atom_sites_fract_tran_vector_3*** (*cif_core.dic 2.0.1*)
The [3] element of the three-element vector used to transform Cartesian coordinates in the ATOM_SITE category to fractional coordinates in the same category. The axial alignments of this transformation are described in **_atom_sites.Cartn_transform_axes**. The 3 × 3 rotation is defined in **_atom_sites.fract_transf_matrix**[][].

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{fractional}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

**[atom_sites]**

**_atom_sites.solution_hydrogens** (*ucode*)
***_atom_sites_solution_hydrogens*** (*cif_core.dic 2.0.1*)
This code identifies the method used to locate the hydrogen atoms.

*Note:* This data item would not in general be used in a macromolecular data block.

The data value must be one of the following:

| | |
|---|---|
| `difmap` | difference Fourier map |
| `vecmap` | real-space vector search |
| `heavy` | heavy-atom method |
| `direct` | structure-invariant direct methods |
| `geom` | inferred from neighbouring sites |
| `disper` | anomalous-dispersion techniques |
| `isomor` | isomorphous structure methods |

**[atom_sites]**

**_atom_sites.solution_primary** (*ucode*)
***_atom_sites_solution_primary*** (*cif_core.dic 2.0.1*)
This code identifies the method used to locate the initial atom sites.

*Note:* This data item would not in general be used in a macromolecular data block.

The data value must be one of the following:

| | |
|---|---|
| `difmap` | difference Fourier map |
| `vecmap` | real-space vector search |
| `heavy` | heavy-atom method |
| `direct` | structure-invariant direct methods |
| `geom` | inferred from neighbouring sites |
| `disper` | anomalous-dispersion techniques |
| `isomor` | isomorphous structure methods |

**[atom_sites]**

**_atom_sites.solution_secondary** (*ucode*)
***_atom_sites_solution_secondary*** (*cif_core.dic 2.0.1*)
This code identifies the method used to locate the non-hydrogen-atom sites not found by **_atom_sites.solution_primary**.

*Note:* This data item would not in general be used in a macromolecular data block.

The data value must be one of the following:

| | |
|---|---|
| `difmap` | difference Fourier map |
| `vecmap` | real-space vector search |
| `heavy` | heavy-atom method |
| `direct` | structure-invariant direct methods |
| `geom` | inferred from neighbouring sites |
| `disper` | anomalous-dispersion techniques |
| `isomor` | isomorphous structure methods |

**[atom_sites]**

**_atom_sites.special_details** (*text*)
***_atom_sites_special_details*** (*cif_core.dic 2.3*)
Additional information about the atomic coordinates not coded elsewhere in the CIF.

**[atom_sites]**

## ATOM_SITES_ALT

Data items in the ATOM_SITES_ALT category record details about the structural ensembles that should be generated from atom sites or groups of atom sites that are modelled in alternative conformations in this data block.

Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_sites_alt.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_sites_alt.id
_atom_sites_alt.details
 .
; Atom sites with the alternative ID set to null are not
  modeled in alternative conformations
;
 1
; Atom sites with the alternative ID set to 1 have been
  modeled in alternative conformations with respect to atom
  sites marked with alternative ID 2. The conformations of
  amino-acid side chains and solvent atoms with alternative
  ID set to 1 correlate with the conformation of the
  inhibitor marked with alternative ID 1. They have been
  given an occupancy of 0.58 to match the occupancy assigned
  to the inhibitor.
;
```

```
 2
; Atom sites with the alternative ID set to 2 have been
  modeled in alternative conformations with respect to atom
  sites marked with alternative ID 1. The conformations of
  amino-acid side chains and solvent atoms with alternative
  ID set to 2 correlate with the conformation of the
  inhibitor marked with alternative ID 2. They have been
  given an occupancy of 0.42 to match the occupancy assigned
  to the inhibitor.
;
 3
; Atom sites with the alternative ID set to 3 have been
  modeled in alternative conformations with respect to
  atoms marked with alternative ID 4. The conformations of
  amino-acid side chains and solvent atoms with alternative
  ID set to 3 do not correlate with the conformation of the
  inhibitor. These atom sites have arbitrarily been given
  an occupancy of 0.50.
;
 4
; Atom sites with the alternative ID set to 4 have been
  modeled in alternative conformations with respect to
  atoms marked with alternative ID 3. The conformations of
  amino-acid side chains and solvent atoms with alternative
  ID set to 4 do not correlate with the conformation of the
  inhibitor. These atom sites have arbitrarily been given
  an occupancy of 0.50.
;
```

**_atom_sites_alt.details** (*text*)

A description of special aspects of the modelling of atoms in alternative conformations.

[atom_sites_alt]

***_atom_sites_alt.id** (*code*)

The value of **_atom_sites_alt.id** must uniquely identify a record in the ATOM_SITES_ALT list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_site.label_alt_id***,
***_atom_sites_alt_gen.alt_id***,
***_geom_angle.atom_site_label_alt_id_1***,
***_geom_angle.atom_site_label_alt_id_2***,
***_geom_angle.atom_site_label_alt_id_3***,
***_geom_bond.atom_site_label_alt_id_1***,
***_geom_bond.atom_site_label_alt_id_2***,
***_geom_contact.atom_site_label_alt_id_1***,
***_geom_contact.atom_site_label_alt_id_2***,
***_geom_hbond.atom_site_label_alt_id_A***,
***_geom_hbond.atom_site_label_alt_id_D***,
***_geom_hbond.atom_site_label_alt_id_H***,
***_geom_torsion.atom_site_label_alt_id_1***,
***_geom_torsion.atom_site_label_alt_id_2***,
***_geom_torsion.atom_site_label_alt_id_3***,
***_geom_torsion.atom_site_label_alt_id_4***,
***_struct_conn.ptnr1_label_alt_id***,
***_struct_conn.ptnr2_label_alt_id***,
***_struct_mon_nucl.label_alt_id***,
***_struct_mon_prot.label_alt_id***,
***_struct_mon_prot_cis.label_alt_id***,
***_struct_ncs_dom_lim.beg_label_alt_id***,
***_struct_ncs_dom_lim.end_label_alt_id***,
***_struct_site_gen.label_alt_id***.

Examples: 'orientation 1', 'molecule abc'. [atom_sites_alt]

## ATOM_SITES_ALT_ENS

Data items in the ATOM_SITES_ALT_ENS category record details about the ensemble structure generated from atoms with various alternative conformation IDs.

Category group(s): **inclusive_group**
**atom_group**

Category key(s): **_atom_sites_alt_ens.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_sites_alt_ens.id
_atom_sites_alt_ens.details
 'Ensemble 1-A'
; The inhibitor binds to the enzyme in two, roughly twofold
  symmetric alternative conformations.

  This conformational ensemble includes the more populated
  conformation of the inhibitor (ID=1) and the amino-acid
  side chains and solvent structure that correlate with this
  inhibitor conformation.

  Also included are one set (ID=3) of side chains with
  alternative conformations when the conformations are not
  correlated with the inhibitor conformation.
;
 'Ensemble 1-B'
; The inhibitor binds to the enzyme in two, roughly twofold
  symmetric alternative conformations.

  This conformational ensemble includes the more populated
  conformation of the inhibitor (ID=1) and the amino-acid
  side chains and solvent structure that correlate with
  this inhibitor conformation.

  Also included are one set (ID=4) of side chains with
  alternative conformations when the conformations are not
  correlated with the inhibitor conformation.
;
 'Ensemble 2-A'
; The inhibitor binds to the enzyme in two, roughly twofold
  symmetric alternative conformations.

  This conformational ensemble includes the less populated
  conformation of the inhibitor (ID=2) and the amino-acid
  side chains and solvent structure that correlate with this
  inhibitor conformation.

  Also included are one set (ID=3) of side chains with
  alternative conformations when the conformations are not
  correlated with the inhibitor conformation.
;
 'Ensemble 2-B'
; The inhibitor binds to the enzyme in two, roughly twofold
  symmetric alternative conformations.

  This conformational ensemble includes the less populated
  conformation of the inhibitor (ID=2) and the amino-acid
  side chains and solvent structure that correlate with this
  inhibitor conformation.

  Also included are one set (ID=4) of side chains with
  alternative conformations when the conformations are not
  correlated with the inhibitor conformation.
;
```

**_atom_sites_alt_ens.details** (*text*)

A description of special aspects of the ensemble structure generated from atoms with various alternative IDs.

[atom_sites_alt_ens]

***_atom_sites_alt_ens.id** (*code*)

The value of **_atom_sites_alt_ens.id** must uniquely identify a record in the ATOM_SITES_ALT_ENS list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_sites_alt_gen.ens_id***. [atom_sites_alt_ens]

## ATOM_SITES_ALT_GEN

Data items in the ATOM_SITES_ALT_GEN category record details about the interpretation of multiple conformations in the structure.

Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_sites_alt_gen.ens_id**
**_atom_sites_alt_gen.alt_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_sites_alt_gen.ens_id
_atom_sites_alt_gen.alt_id
 'Ensemble 1-A'  .
 'Ensemble 1-A'  1
 'Ensemble 1-A'  3
 'Ensemble 1-B'  .
 'Ensemble 1-B'  1
 'Ensemble 1-B'  4
 'Ensemble 2-A'  .
 'Ensemble 2-A'  2
 'Ensemble 2-A'  3
 'Ensemble 2-B'  .
 'Ensemble 2-B'  2
 'Ensemble 2-B'  4
```

***_atom_sites_alt_gen.alt_id**
This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_atom_sites_alt_gen.ens_id**
This data item is a pointer to **_atom_sites_alt_ens.id** in the ATOM_SITES_ALT_ENS category.

## ATOM_SITES_FOOTNOTE

Data items in the ATOM_SITES_FOOTNOTE category record detailed comments about an atom site or a group of atom sites.

Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_sites_footnote.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_sites_footnote.id
_atom_sites_footnote.text
  1
; The inhibitor binds to the enzyme in two alternative
  orientations. The two orientations have been assigned
  alternative IDs *1* and *2*.
;
  2
; Side chains of these residues adopt alternative
  orientations that correlate with the alternative
  orientations of the inhibitor.
  Side chains with alternative ID *1* and occupancy 0.58
  correlate with inhibitor orientation *1*.
  Side chains with alternative ID *2* and occupancy 0.42
  correlate with inhibitor orientation *2*.
;
  3
; The positions of these water molecules correlate with
  the alternative orientations of the inhibitor.
  Water molecules with alternative ID *1* and occupancy 0.58
  correlate with inhibitor orientation *1*.
  Water molecules with alternative ID *2* and occupancy 0.42
  correlate with inhibitor orientation *2*.
;
  4
; Side chains of these residues adopt alternative
  orientations that do not correlate with the alternative
  orientation of the inhibitor.
;
  5
; The positions of these water molecules correlate with
  alternative orientations of amino-acid side chains that
  do not correlate with alternative orientations of the
  inhibitor.
;
```

***_atom_sites_footnote.id** (*code*)
A code that identifies the footnote.

*The following item(s) have an equivalent role in their respective categories:*
***_atom_site.footnote_id***.

Examples: 'a', 'b', '1', '2'. **[atom_sites_footnote]**

**_atom_sites_footnote.text** (*text*)
The text of the footnote. Footnotes are used to describe an atom site or a group of atom sites in the ATOM_SITE list. For example, footnotes may be used to indicate atoms for which the electron density is very weak, or atoms for which static disorder has been modelled.

**[atom_sites_footnote]**

## ATOM_TYPE

Data items in the ATOM_TYPE category record details about the properties of the atoms that occupy the atom sites, such as the atomic scattering factors.

Category group(s): **inclusive_group**
**atom_group**
Category key(s): **_atom_type.symbol**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_atom_type.symbol
_atom_type.oxidation_number
_atom_type.scat_Cromer_Mann_a1
_atom_type.scat_Cromer_Mann_a2
_atom_type.scat_Cromer_Mann_a3
_atom_type.scat_Cromer_Mann_a4
_atom_type.scat_Cromer_Mann_b1
_atom_type.scat_Cromer_Mann_b2
_atom_type.scat_Cromer_Mann_b3
_atom_type.scat_Cromer_Mann_b4
_atom_type.scat_Cromer_Mann_c
  C   0   2.31000  20.8439    1.02000   10.2075
          1.58860   0.568700  0.865000  51.6512      0.21560
  N   0  12.2126    0.005700  3.13220    9.89330
          2.01250  28.9975    1.16630    0.582600  -11.529
  O   0   3.04850  13.2771    2.28680    5.70110
          1.54630   0.323900  0.867000  32.9089      0.250800
  S   0   6.90530   1.46790   5.20340   22.2151
          1.43790   0.253600  1.58630   56.1720      0.866900
  CL -1  18.2915    0.006600  7.20840    1.17170
          6.53370  19.5424    2.33860   60.4486    -16.378
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 276–2277].*

```
loop_
_atom_type.symbol
_atom_type.oxidation_number
_atom_type.number_in_cell
_atom_type.scat_dispersion_real
_atom_type.scat_dispersion_imag
_atom_type.scat_source
 C  0  72  .017  .009  International_Tables_Vol_IV_Table_2.2B
 H  0  100  0     0    International_Tables_Vol_IV_Table_2.2B
 O  0  12  .047  .032  International_Tables_Vol_IV_Table_2.2B
 N  0  4   .029  .018  International_Tables_Vol_IV_Table_2.2B
```

**_atom_type.analytical_mass_percent** (*float*)
*_atom_type_analytical_mass_%* (*cif_core.dic 2.0.1*)
Mass percentage of this atom type derived from chemical analysis.
The permitted range is $[0.0, \infty)$. **[atom_type]**

**_atom_type.description** (*text*)
*_atom_type_description* (*cif_core.dic 2.0.1*)
A description of the atom(s) designated by this atom type. In most cases, this is the element name and oxidation state of a single atom species. For disordered or nonstoichiometric structures it will describe a combination of atom species.
Examples: '`deuterium`', '`0.34Fe+0.66Ni`'. **[atom_type]**

**_atom_type.number_in_cell** (*int*)
*_atom_type_number_in_cell* (*cif_core.dic 2.0.1*)
Total number of atoms of this atom type in the unit cell.
The permitted range is $[0, \infty)$. **[atom_type]**

**_atom_type.oxidation_number** (*int*)
*_atom_type_oxidation_number* (*cif_core.dic 2.0.1*)
Formal oxidation state of this atom type in the structure.
The permitted range is $[-8, 8]$. Where no value is given, the assumed value is '`0`'.
**[atom_type]**

**_atom_type.radius_bond** (*float*)
*_atom_type_radius_bond* (*cif_core.dic 2.0.1*)
The effective intramolecular bonding radius in ångströms of this atom type.
The permitted range is [0.0, 5.0]. **[atom_type]**

**_atom_type.radius_contact** (*float*)
*_atom_type_radius_contact* (*cif_core.dic 2.0.1*)
The effective intermolecular bonding radius in ångströms of this atom type.
The permitted range is [0.0, 5.0]. **[atom_type]**

**_atom_type.scat_Cromer_Mann_a1** (*float*)
*_atom_type_scat_Cromer_Mann_a1* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $a_1$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_a2** (*float*)
*_atom_type_scat_Cromer_Mann_a2* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $a_2$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_a3** (*float*)
*_atom_type_scat_Cromer_Mann_a3* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $a_3$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_a4** (*float*)
*_atom_type_scat_Cromer_Mann_a4* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $a_4$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_b1** (*float*)
*_atom_type_scat_Cromer_Mann_b1* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $b_1$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_b2** (*float*)
*_atom_type_scat_Cromer_Mann_b2* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $b_2$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_b3** (*float*)
*_atom_type_scat_Cromer_Mann_b3* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $b_3$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_b4** (*float*)
*_atom_type_scat_Cromer_Mann_b4* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $b_4$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_Cromer_Mann_c** (*float*)
*_atom_type_scat_Cromer_Mann_c* (*cif_core.dic 2.0.1*)
The Cromer–Mann scattering-factor coefficient $c$ used to calculate the scattering factors for this atom type.

References: *International Tables for X-ray Crystallography* (1974). Vol. IV, Table 2.2B; *International Tables for Crystallography* (2004). Vol. C, Tables 6.1.1.4 and 6.1.1.5.
**[atom_type]**

**_atom_type.scat_dispersion_imag** (*float*)
*_atom_type_scat_dispersion_imag* (*cif_core.dic 2.0.1*)
The imaginary component of the anomalous-dispersion scattering factor, $f''$, in electrons for this atom type and the radiation identified by **_diffrn_radiation_wavelength.id**.
**[atom_type]**

**_atom_type.scat_dispersion_real** (*float*)
*_atom_type_scat_dispersion_real* (*cif_core.dic 2.0.1*)
The real component of the anomalous-dispersion scattering factor, $f'$, in electrons for this atom type and the radiation identified by **_diffrn_radiation_wavelength.id**.
**[atom_type]**

### _atom_type.scat_dispersion_source (*text*)

***_atom_type_scat_dispersion_source*** (*cif_core.dic 2.3*)

Reference to the source of the real and imaginary dispersion corrections for scattering factors used for this atom type.

Example: 'International Tables Vol. IV Table 2.3.1'. **[atom_type]**

### _atom_type.scat_length_neutron (*text*)

***_atom_type_scat_length_neutron*** (*cif_core.dic 2.0.1*)

The bound coherent scattering length in femtometres for the atom type at the isotopic composition used for the diffraction experiment.

**[atom_type]**

### _atom_type.scat_source (*text*)

***_atom_type_scat_source*** (*cif_core.dic 2.0.1*)

Reference to the source of the scattering factors or scattering lengths used for this atom type.

Example: 'International Tables Vol. IV Table 2.4.6B'. **[atom_type]**

### _atom_type.scat_versus_stol_list (*text*)

***_atom_type_scat_versus_stol_list*** (*cif_core.dic 2.0.1*)

A table of scattering factors as a function of $(\sin\theta)/\lambda$. This table should be well commented to indicate the items present. Regularly formatted lists are strongly recommended.

**[atom_type]**

### *_atom_type.symbol (*code*)

***_atom_type_symbol*** (*cif_core.dic 2.0.1*)

The code used to identify the atom species (singular or plural) representing this atom type. Normally this code is the element symbol. The code may be composed of any character except an underscore with the additional proviso that digits designate an oxidation state and must be followed by a + or - character.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_site.type_symbol***,
***_atom_site_anisotrop.type_symbol***,
***_chemical_conn_atom.type_symbol***,
***_chem_comp_atom.type_symbol***,
***_phasing_MIR_der_site.atom_type_symbol***.

Examples: 'C', 'Cu2+', 'H(SDS)', 'dummy', 'FeNi'. **[atom_type]**

## AUDIT

Data items in the AUDIT category record details about the creation and subsequent updating of the data block. Note that these items apply only to the creation and updating of the data block, and should not be confused with the data items in the JOURNAL category that record different stages in the publication of the material in the data block.

Category group(s): **inclusive_group**
**audit_group**
Category key(s): **_audit.revision_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_audit.revision_id                 1
_audit.creation_date              '1992-12-08'

_audit.creation_method
; Created by hand from PDB entry 5HVP, from the J. Biol.
  Chem. paper describing this structure and from
  laboratory records
;

_audit.update_record
; 1992-12-09  adjusted to reflect comments from B. McKeever
  1992-12-10  adjusted to reflect comments from H. Berman
  1992-12-12  adjusted to reflect comments from K. Watenpaugh
;
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C**47**, 2276–2277].*

```
_audit.creation_date              1991-03-20
_audit.creation_method    from_xtal_archive_file_using_CIFIO
_audit.update_record
; 1991-04-09  text and data added by Tony Willis.
  1991-04-15  rec'd by co-editor as manuscript HL0007.
  1991-04-17  adjustments based on first referee report.
  1991-04-18  adjustments based on second referee report.
;
```

### _audit.creation_date (*yyyy-mm-dd*)

***_audit_creation_date*** (*cif_core.dic 2.0.1*)

A date that the data block was created. The date format is *yyyy-mm-dd*.

Example: '1990-07-12'. **[audit]**

### _audit.creation_method (*text*)

***_audit_creation_method*** (*cif_core.dic 2.0.1*)

A description of how data were entered into the data block.

Example: 'spawned by the program QBEE'. **[audit]**

### *_audit.revision_id (*code*)

The value of **_audit.revision_id** must uniquely identify a record in the AUDIT list.

Example: 'rev1'. **[audit]**

### _audit.update_record (*text*)

***_audit_update_record*** (*cif_core.dic 2.0.1*)

A record of any changes to the data block. The update format is a date (*yyyy-mm-dd*) followed by a description of the changes. The latest update entry is added to the bottom of this record.

Example: '1990-07-15 Updated by the Co-editor'. **[audit]**

## AUDIT_AUTHOR

Data items in the AUDIT_AUTHOR category record details about the author(s) of the data block.

Category group(s): **inclusive_group**
**audit_group**
Category key(s): **_audit_author.name**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_audit_author.name
_audit_author.address
 'Fitzgerald, Paula M.D.'
; Department of Biophysical Chemistry
  Merck Research Laboratories
  P. O. Box 2000, Ry80M203
  Rahway, New Jersey  07065
  USA
;
 'McKeever, Brian M.'
; Department of Biophysical Chemistry
  Merck Research Laboratories
  P. O. Box 2000, Ry80M203
  Rahway, New Jersey  07065
  USA
;
 'Van Middlesworth, J.F.'
; Department of Biophysical Chemistry
  Merck Research Laboratories
  P. O. Box 2000, Ry80M203
  Rahway, New Jersey  07065
  USA
;
 'Springer, James P.'
; Department of Biophysical Chemistry
  Merck Research Laboratories
  P. O. Box 2000, Ry80M203
  Rahway, New Jersey  07065
  USA
;
```

### _audit_author.address (*text*)

***_audit_author_address*** (*cif_core.dic 2.0.1*)

The address of an author of this data block. If there are multiple authors, **_audit_author.address** is looped with **_audit_author.name**.

Example:

```
; Department
  Institute
  Street
  City and postcode
  COUNTRY
;
```

**[audit_author]**

### *_audit_author.name (*line*)

***_audit_author_name*** (*cif_core.dic 2.0.1*)

The name of an author of this data block. If there are multiple authors, **_audit_author.name** is looped with **_audit_author.address**. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).

Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[audit_author]**

## AUDIT_CONFORM

Data items in the AUDIT_CONFORM category describe the dictionary versions against which the data names appearing in the current data block are conformant.

Category group(s): **inclusive_group**
**audit_group**

Category key(s): **_audit_conform.dict_name**
**_audit_conform.dict_version**

*Example 1 – any file conforming to the current CIF core dictionary.*

```
_audit_conform.dict_name        cif_core.dic
_audit_conform.dict_version     2.3.1
_audit_conform.dict_location
     ftp://ftp.iucr.org/pub/cif_core.2.3.1.dic
```

### _audit_conform.dict_location (*text*)

***_audit_conform_dict_location*** (*cif_core.dic 2.0.1*)

A file name or uniform resource locator (URL) for the dictionary to which the current data block conforms.

**[audit_conform]**

### _audit_conform.dict_name (*text*)

***_audit_conform_dict_name*** (*cif_core.dic 2.0.1*)

The string identifying the highest-level dictionary defining data names used in this file.

**[audit_conform]**

### _audit_conform.dict_version (*text*)

***_audit_conform_dict_version*** (*cif_core.dic 2.0.1*)

The version number of the dictionary to which the current data block conforms.

**[audit_conform]**

## AUDIT_CONTACT_AUTHOR

Data items in the AUDIT_CONTACT_AUTHOR category record details about the name and address of the author to be contacted concerning the content of this data block.

Category group(s): **inclusive_group**
**audit_group**

Category key(s): **_audit_contact_author.name**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_audit_contact_author.name   'Fitzgerald, Paula M.D.'
_audit_contact_author.address
; Department of Biophysical Chemistry
  Merck Research Laboratories
  PO Box 2000, Ry80M203
  Rahway, New Jersey 07065
  USA
;
_audit_contact_author.phone  '1(908)5945510'
_audit_contact_author.fax    '1(908)5946645'
_audit_contact_author.email  'paula_fitzgerald@merck.com'
```

### _audit_contact_author.address (*text*)

***_audit_contact_author_address*** (*cif_core.dic 2.0.1*)

The mailing address of the author of the data block to whom correspondence should be addressed.

Example:

```
; Department
  Institute
  Street
  City and postcode
  COUNTRY
;
```

**[audit_contact_author]**

### _audit_contact_author.email (*line*)

***_audit_contact_author_email*** (*cif_core.dic 2.0.1*)

The electronic mail address of the author of the data block to whom correspondence should be addressed, in a form recognizable to international networks. The format of e-mail addresses is given in Section 3.4, *Address Specification*, of *Internet Message Format*, RFC 2822, P. Resnick (Editor), Network Standards Group, April 2001.

Examples: 'name@host.domain.country', 'bm@iucr.org'.

**[audit_contact_author]**

### _audit_contact_author.fax (*line*)

***_audit_contact_author_fax*** (*cif_core.dic 2.0.1*)

The facsimile telephone number of the author of the data block to whom correspondence should be addressed. The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces.

Examples: '12(34)9477334', '12()349477334'. **[audit_contact_author]**

### *_audit_contact_author.name (*line*)

***_audit_contact_author_name*** (*cif_core.dic 2.0.1*)

The name of the author of the data block to whom correspondence should be addressed. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).

Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[audit_contact_author]**

### _audit_contact_author.phone (*line*)

***_audit_contact_author_phone*** (*cif_core.dic 2.0.1*)

The telephone number of the author of the data block to whom correspondence should be addressed. The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number and any extension number prefixed by 'x', with no spaces.

Examples: '12(34)9477330', '12()349477330', '12(34)9477330x5543'.

**[audit_contact_author]**

## AUDIT_LINK

Data items in the AUDIT_LINK category record details about the relationships between data blocks in the current CIF.

Category key(s): `_audit_link.block_code`
`_audit_link.block_description`

*Example 1 – multiple structure paper, as illustrated in A Guide to CIF for Authors (1995). IUCr: Chester.*

```
loop_
_audit_link.block_code
_audit_link.block_description
   .         'discursive text of paper with two structures'
   morA_(1)  'structure 1 of 2'
   morA_(2)  'structure 2 of 2'
```

*Example 2 – example file for the one-dimensional incommensurately modulated structure of $K_2SeO_4$.*

```
loop_
_audit_link.block_code
_audit_link.block_description
 .        'publication details'
 KSE_COM  'experimental data common to ref./mod. structures'
 KSE_REF  'reference structure'
 KSE_MOD  'modulated structure'
```

### *_audit_link.block_code (*code*)

*_audit_link_block_code* (*cif_core.dic 2.3*)

The value of `_audit_block.code` associated with a data block in the current file related to the current data block. The special value '.' may be used to refer to the current data block for completeness.

**[audit_link]**

### *_audit_link.block_description (*text*)

*_audit_link_block_description* (*cif_core.dic 2.3*)

A textual description of the relationship of the referenced data block to the current one.

**[audit_link]**

## CELL

Data items in the CELL category record details about the crystallographic cell parameters.

Category group(s): `inclusive_group`
`cell_group`

Category key(s): `_cell.entry_id`

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_cell.entry_id                   '5HVP'
_cell.length_a                   58.39
_cell.length_a_esd                0.05
_cell.length_b                   86.70
_cell.length_b_esd                0.12
_cell.length_c                   46.27
_cell.length_c_esd                0.06
_cell.angle_alpha                90.00
_cell.angle_beta                 90.00
_cell.angle_gamma                90.00
_cell.volume                     234237
_cell.details
; The cell parameters were refined every twenty frames during
  data integration. The cell lengths given are the mean of
  55 such refinements; the esds given are the root mean
  square deviations of these 55 observations from that mean.
;
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276–2277].*

```
_cell.length_a                    5.959
_cell.length_a_esd                0.001
_cell.length_b                   14.956
_cell.length_b_esd                0.001
_cell.length_c                   19.737
_cell.length_c_esd                0.003
_cell.angle_alpha                90.0
_cell.angle_beta                 90.0
_cell.angle_gamma                90.0
_cell.volume                   1759.0
_cell.volume_esd                  0.3
```

### `_cell.angle_alpha` (*float, su*)

*_cell_angle_alpha* (*cif_core.dic 2.0.1*)

Unit-cell angle $\alpha$ of the reported structure in degrees.

The permitted range is [0.0, 180.0].

Related item: `_cell.angle_alpha_esd` (associated esd). Where no value is given, the assumed value is '`90.0`'. **[cell]**

### `_cell.angle_alpha_esd` (*float*)

The standard uncertainty (estimated standard deviation) of `_cell.angle_alpha`.

Related item: `_cell.angle_alpha` (associated value). **[cell]**

### `_cell.angle_beta` (*float, su*)

*_cell_angle_beta* (*cif_core.dic 2.0.1*)

Unit-cell angle $\beta$ of the reported structure in degrees.

The permitted range is [0.0, 180.0].

Related item: `_cell.angle_beta_esd` (associated esd). Where no value is given, the assumed value is '`90.0`'. **[cell]**

### `_cell.angle_beta_esd` (*float*)

The standard uncertainty (estimated standard deviation) of `_cell.angle_beta`.

Related item: `_cell.angle_beta` (associated value). **[cell]**

### `_cell.angle_gamma` (*float, su*)

*_cell_angle_gamma* (*cif_core.dic 2.0.1*)

Unit-cell angle $\gamma$ of the reported structure in degrees.

The permitted range is [0.0, 180.0].

Related item: `_cell.angle_gamma_esd` (associated esd). Where no value is given, the assumed value is '`90.0`'. **[cell]**

### `_cell.angle_gamma_esd` (*float*)

The standard uncertainty (estimated standard deviation) of `_cell.angle_gamma`.

Related item: `_cell.angle_gamma` (associated value). **[cell]**

### `_cell.details` (*text*)

*_cell_special_details* (*cif_core.dic 2.0.1*)

A description of special aspects of the cell choice, noting possible alternative settings.

Examples: '`pseudo-orthorhombic`',
'`standard setting from 45 deg rotation around c`'. **[cell]**

### *`_cell.entry_id`

This data item is a pointer to `_entry.id` in the ENTRY category.

### `_cell.formula_units_Z` (*int*)

*_cell_formula_units_Z* (*cif_core.dic 2.0.1*)

The number of the formula units in the unit cell as specified by `_chemical_formula.structural`, `_chemical_formula.moiety` or `_chemical_formula.sum`.

The permitted range is $[1, \infty)$. **[cell]**

**_cell.length_a** (*float, su*)
**_cell_length_a** (*cif_core.dic 2.0.1*)
Unit-cell length $a$ corresponding to the structure reported in ångströms.
The permitted range is $[0.0, \infty)$.
Related item: **_cell.length_a_esd** (associated esd). **[cell]**

**_cell.length_a_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell.length_a**.
Related item: **_cell.length_a** (associated value). **[cell]**

**_cell.length_b** (*float, su*)
**_cell_length_b** (*cif_core.dic 2.0.1*)
Unit-cell length $b$ corresponding to the structure reported in ångströms.
The permitted range is $[0.0, \infty)$.
Related item: **_cell.length_b_esd** (associated esd). **[cell]**

**_cell.length_b_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell.length_b**.
Related item: **_cell.length_b** (associated value). **[cell]**

**_cell.length_c** (*float, su*)
**_cell_length_c** (*cif_core.dic 2.0.1*)
Unit-cell length $c$ corresponding to the structure reported in ångströms.
The permitted range is $[0.0, \infty)$.
Related item: **_cell.length_c_esd** (associated esd). **[cell]**

**_cell.length_c_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell.length_c**.
Related item: **_cell.length_c** (associated value). **[cell]**

**_cell.reciprocal_angle_alpha** (*float, su*)
**_cell_reciprocal_angle_alpha** (*cif_core.dic 2.3*)
The angle $\alpha^*$ defining the reciprocal cell in degrees. $\alpha^*$, $\beta^*$ and $\gamma*$ are related to the angles in the real cell by

$$\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/(\sin\beta\sin\gamma),$$
$$\cos\beta^* = (\cos\gamma\cos\alpha - \cos\beta)/(\sin\gamma\sin\alpha),$$
$$\cos\gamma^* = (\cos\alpha\cos\beta - \cos\gamma)/(\sin\alpha\sin\beta).$$

Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.
The permitted range is [0.0, 180.0].
Related item: **_cell.reciprocal_angle_alpha_esd** (associated esd). Where no value is given, the assumed value is '90.0'. **[cell]**

**_cell.reciprocal_angle_alpha_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_angle_alpha**.
Related item: **_cell.reciprocal_angle_alpha** (associated value). **[cell]**

**_cell.reciprocal_angle_beta** (*float, su*)
**_cell_reciprocal_angle_beta** (*cif_core.dic 2.3*)
The angle $\beta^*$ defining the reciprocal cell in degrees. $\alpha^*$, $\beta^*$ and $\gamma^*$ are related to the angles in the real cell by

$$\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/(\sin\beta\sin\gamma),$$
$$\cos\beta^* = (\cos\gamma\cos\alpha - \cos\beta)/(\sin\gamma\sin\alpha),$$
$$\cos\gamma^* = (\cos\alpha\cos\beta - \cos\gamma)/(\sin\alpha\sin\beta).$$

Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.
The permitted range is [0.0, 180.0].
Related item: **_cell.reciprocal_angle_beta_esd** (associated esd). Where no value is given, the assumed value is '90.0'. **[cell]**

**_cell.reciprocal_angle_beta_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_angle_beta**.
Related item: **_cell.reciprocal_angle_beta** (associated value). **[cell]**

**_cell.reciprocal_angle_gamma** (*float, su*)
**_cell_reciprocal_angle_gamma** (*cif_core.dic 2.3*)
The angle $\gamma^*$ defining the reciprocal cell in degrees. $\alpha^*$, $\beta^*$ and $\gamma^*$ are related to the angles in the real cell by

$$\cos\alpha^* = (\cos\beta\cos\gamma - \cos\alpha)/(\sin\beta\sin\gamma),$$
$$\cos\beta^* = (\cos\gamma\cos\alpha - \cos\beta)/(\sin\gamma\sin\alpha),$$
$$\cos\gamma^* = (\cos\alpha\cos\beta - \cos\gamma)/(\sin\alpha\sin\beta).$$

Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.
The permitted range is [0.0, 180.0].
Related item: **_cell.reciprocal_angle_gamma_esd** (associated esd). Where no value is given, the assumed value is '90.0'. **[cell]**

**_cell.reciprocal_angle_gamma_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_angle_gamma**.
Related item: **_cell.reciprocal_angle_gamma** (associated value). **[cell]**

**_cell.reciprocal_length_a** (*float, su*)
**_cell_reciprocal_length_a** (*cif_core.dic 2.3*)
The reciprocal-cell length $a^*$ in inverse ångströms. $a^*$, $b^*$ and $c^*$ are related to the lengths in the real cell by

$$a^* = bc\sin\alpha/V,$$
$$b^* = ca\sin\beta/V,$$
$$c^* = ab\sin\gamma/V,$$

where $V$ is the cell volume.
Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.
The permitted range is $[0.0, \infty)$.
Related item: **_cell.reciprocal_length_a_esd** (associated esd). **[cell]**

**_cell.reciprocal_length_a_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_length_a**.
Related item: **_cell.reciprocal_length_a** (associated value). **[cell]**

**_cell.reciprocal_length_b** (*float, su*)
***_cell_reciprocal_length_b*** (*cif_core.dic 2.3*)
The reciprocal-cell length $b^*$ in inverse ångströms. $a^*$, $b^*$ and $c^*$ are related to the lengths in the real cell by

$$a^* = bc\sin\alpha/V,$$
$$b^* = ca\sin\beta/V,$$
$$c^* = ab\sin\gamma/V,$$

where $V$ is the cell volume.

Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.

The permitted range is $[0.0, \infty)$.

Related item: **_cell.reciprocal_length_b_esd** (associated esd). **[cell]**

**_cell.reciprocal_length_b_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_length_b**.

Related item: **_cell.reciprocal_length_b** (associated value). **[cell]**

**_cell.reciprocal_length_c** (*float, su*)
***_cell_reciprocal_length_c*** (*cif_core.dic 2.3*)
The reciprocal-cell length $c^*$ in inverse ångströms. $a^*$, $b^*$ and $c^*$ are related to the lengths in the real cell by

$$a^* = bc\sin\alpha/V,$$
$$b^* = ca\sin\beta/V,$$
$$c^* = ab\sin\gamma/V,$$

where $V$ is the cell volume.

Reference: Buerger, M. J. (1942). *X-ray Crystallography*, p. 360. New York: John Wiley & Sons Inc.

The permitted range is $[0.0, \infty)$.

Related item: **_cell.reciprocal_length_c_esd** (associated esd). **[cell]**

**_cell.reciprocal_length_c_esd** (*float*)
The estimated standard deviation of **_cell.reciprocal_length_c**.

Related item: **_cell.reciprocal_length_c** (associated value). **[cell]**

**_cell.volume** (*float, su*)
***_cell_volume*** (*cif_core.dic 2.0.1*)
Cell volume $V$ in ångströms cubed.

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2},$$

where $a$ = **_cell.length_a**, $b$ = **_cell.length_b**, $c$ = **_cell.length_c**, $\alpha$ = **_cell.angle_alpha**, $\beta$ = **_cell.angle_beta** and $\gamma$ = **_cell.angle_gamma**.

The permitted range is $[0.0, \infty)$.

Related item: **_cell.volume_esd** (associated esd). **[cell]**

**_cell.volume_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell.volume**.

Related item: **_cell.volume** (associated value). **[cell]**

**_cell.Z_PDB** (*int*)
The number of the polymeric chains in a unit cell. In the case of heteropolymers, $Z$ is the number of occurrences of the most populous chain. This data item is provided for compatibility with the original Protein Data Bank format, and only for that purpose.

The permitted range is $[1, \infty)$. **[cell]**

## CELL_MEASUREMENT

Data items in the CELL_MEASUREMENT category record details about the measurement of the crystallographic cell parameters.

Category group(s): **inclusive_group**
**cell_group**
Category key(s): **_cell_measurement.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_cell_measurement.entry_id            '5HVP'
_cell_measurement.temp                293
_cell_measurement.temp_esd            3
_cell_measurement.theta_min           11
_cell_measurement.theta_max           31
_cell_measurement.wavelength          1.54
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
_cell_measurement.temp                293
_cell_measurement.reflns_used         25
_cell_measurement.theta_min           25
_cell_measurement.theta_max           31
```

***_cell_measurement.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_cell_measurement.pressure** (*float, su*)
***_cell_measurement_pressure*** (*cif_core.dic 2.0.1*)
The pressure in kilopascals at which the unit-cell parameters were measured (not the pressure at which the sample was synthesized).

Related item: **_cell_measurement.pressure_esd** (associated esd).
**[cell_measurement]**

**_cell_measurement.pressure_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell_measurement.pressure**.

Related item: **_cell_measurement.pressure** (associated value).
**[cell_measurement]**

**_cell_measurement.radiation** (*line*)
***_cell_measurement_radiation*** (*cif_core.dic 2.0.1*)
Description of the radiation used to measure the unit-cell data. See also **_cell_measurement.wavelength**.

Examples: 'neutron', 'Cu K\a', 'synchrotron'. **[cell_measurement]**

**_cell_measurement.reflns_used** (*int*)
***_cell_measurement_reflns_used*** (*cif_core.dic 2.0.1*)
The total number of reflections used to determine the unit cell. These reflections may be specified as CELL_MEASUREMENT_REFLN data items.

**[cell_measurement]**

**_cell_measurement.temp** (*float, su*)
***_cell_measurement_temperature*** (*cif_core.dic 2.0.1*)
The temperature in kelvins at which the unit-cell parameters were measured (not the temperature of synthesis).

The permitted range is $[0.0, \infty)$.

Related item: **_cell_measurement.temp_esd** (associated esd).
**[cell_measurement]**

**_cell_measurement.temp_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_cell_measurement.temp**.

Related item: **_cell_measurement.temp** (associated value). **[cell_measurement]**

**_cell_measurement.theta_max** (*float*)
***_cell_measurement_theta_max*** (*cif_core.dic 2.0.1*)
The maximum $\theta$ angle of reflections used to measure the unit cell in degrees.
The permitted range is [0.0, 90.0]. **[cell_measurement]**

**_cell_measurement.theta_min** (*float*)
***_cell_measurement_theta_min*** (*cif_core.dic 2.0.1*)
The minimum $\theta$ angle of reflections used to measure the unit cell in degrees.
The permitted range is [0.0, 90.0]. **[cell_measurement]**

**_cell_measurement.wavelength** (*float*)
***_cell_measurement_wavelength*** (*cif_core.dic 2.0.1*)
The wavelength in ångströms of the radiation used to measure the unit cell. If this is not specified, the wavelength is assumed to be that specified in the category DIFFRN_RADIATION_WAVELENGTH.
The permitted range is $[0.0, \infty)$. **[cell_measurement]**

## CELL_MEASUREMENT_REFLN

Data items in the CELL_MEASUREMENT_REFLN category record details about the reflections used to determine the crystallographic cell parameters. The CELL_MEASUREMENT_REFLN data items would in general be used only for diffractometer data.
Category group(s): **inclusive_group**
**cell_group**
Category key(s): **_cell_measurement_refln.index_h**
**_cell_measurement_refln.index_k**
**_cell_measurement_refln.index_l**

*Example 1 – extracted from the CAD-4 listing of $Rb_2S_2O_6$ at room temperature (unpublished).*

```
loop_
_cell_measurement_refln.index_h
_cell_measurement_refln.index_k
_cell_measurement_refln.index_l
_cell_measurement_refln.theta
   -2    4    1          8.67
    0    3    2          9.45
    3    0    2          9.46
   -3    4    1          8.93
   -2    1   -2          7.53
   10    0    0         23.77
    0   10    0         23.78
   -5    4    1         11.14
  # - - - - data truncated for brevity - - - -
```

***_cell_measurement_refln.index_h** (*int*)
***_cell_measurement_refln_index_h*** (*cif_core.dic 2.0.1*)
Miller index *h* of a reflection used for measurement of the unit cell.
**[cell_measurement_refln]**

***_cell_measurement_refln.index_k** (*int*)
***_cell_measurement_refln_index_k*** (*cif_core.dic 2.0.1*)
Miller index *k* of a reflection used for measurement of the unit cell.
**[cell_measurement_refln]**

***_cell_measurement_refln.index_l** (*int*)
***_cell_measurement_refln_index_l*** (*cif_core.dic 2.0.1*)
Miller index *l* of a reflection used for measurement of the unit cell.
**[cell_measurement_refln]**

**_cell_measurement_refln.theta** (*float*)
***_cell_measurement_refln_theta*** (*cif_core.dic 2.0.1*)
$\theta$ angle for a reflection used for measurement of the unit cell in degrees.
The permitted range is [0.0, 90.0]. **[cell_measurement_refln]**

## CHEM_COMP

Data items in the CHEM_COMP category give details about each of the chemical components from which the relevant chemical structures can be constructed, such as name, mass or charge. The related categories CHEM_COMP_ATOM, CHEM_COMP_BOND, CHEM_COMP_ANGLE *etc.* describe the detailed geometry of these chemical components.
Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp.id
_chem_comp.model_source
_chem_comp.name
  phe  '1987 Protin/Prolsq Ideals file' phenylalanine
  val  '1987 Protin/Prolsq Ideals file' alanine
# - - - - data truncated for brevity - - - -
```

**_chem_comp.formula** (*text*)
The formula for the chemical component. Formulae are written according to the following rules: (1) Only recognized element symbols may be used. (2) Each element symbol is followed by a 'count' number. A count of '1' may be omitted. (3) A space or parenthesis must separate each cluster of (element symbol + count), but in general parentheses are not used. (4) The order of elements depends on whether carbon is present or not. If carbon is present, the order should be: C, then H, then the other elements in alphabetical order of their symbol. If carbon is not present, the elements are listed purely in alphabetic order of their symbol. This is the 'Hill' system used by *Chemical Abstracts*.
Example: 'C18 H19 N7 O8 S'. **[chem_comp]**

**_chem_comp.formula_weight** (*float*)
Formula mass in daltons of the chemical component.
The permitted range is $[1.0, \infty)$. **[chem_comp]**

***_chem_comp.id** (*ucode*)
The value of **_chem_comp.id** must uniquely identify each item in the CHEM_COMP list. For protein polymer entities, this is the three-letter code for the amino acid. For nucleic acid polymer entities, this is the one-letter code for the base.
*The following item(s) have an equivalent role in their respective categories:*
***_atom_site.label_comp_id***,
***_chem_comp.mon_nstd_parent_comp_id***,
***_chem_comp_atom.comp_id***,
***_chem_comp_chir.comp_id***,
***_chem_comp_chir_atom.comp_id***,
***_chem_comp_plane.comp_id***,
***_chem_comp_plane_atom.comp_id***,
***_entity_poly_seq.mon_id***,
***_chem_comp_angle.comp_id***,
***_chem_comp_bond.comp_id***,
***_chem_comp_tor.comp_id***,
***_chem_comp_tor_value.comp_id***,
***_geom_angle.atom_site_label_comp_id_1***,
***_geom_angle.atom_site_label_comp_id_2***,
***_geom_angle.atom_site_label_comp_id_3***,
***_geom_bond.atom_site_label_comp_id_1***,
***_geom_bond.atom_site_label_comp_id_2***,
***_geom_contact.atom_site_label_comp_id_1***,
***_geom_contact.atom_site_label_comp_id_2***,
***_geom_hbond.atom_site_label_comp_id_A***,
***_geom_hbond.atom_site_label_comp_id_D***,

*_geom_hbond.atom_site_label_comp_id_H*,
*_geom_torsion.atom_site_label_comp_id_1*,
*_geom_torsion.atom_site_label_comp_id_2*,
*_geom_torsion.atom_site_label_comp_id_3*,
*_geom_torsion.atom_site_label_comp_id_4*,
*_struct_conf.beg_label_comp_id*,
*_struct_conf.end_label_comp_id*,
*_struct_conn.ptnr1_label_comp_id*,
*_struct_conn.ptnr2_label_comp_id*,
*_struct_mon_nucl.label_comp_id*,
*_struct_mon_prot.label_comp_id*,
*_struct_mon_prot_cis.label_comp_id*,
*_struct_ncs_dom_lim.beg_label_comp_id*,
*_struct_ncs_dom_lim.end_label_comp_id*,
*_struct_ref_seq_dif.db_mon_id*,
*_struct_ref_seq_dif.mon_id*,
*_struct_sheet_range.beg_label_comp_id*,
*_struct_sheet_range.end_label_comp_id*,
*_struct_site_gen.label_comp_id*.

Examples: 'ala', 'val', 'A', 'C'. **[chem_comp]**

### _chem_comp.model_details (*text*)

A description of special aspects of the generation of the coordinates for the model of the component.

Example: 'geometry idealized but not minimized'. **[chem_comp]**

### _chem_comp.model_erf (*line*)

A pointer to an external reference file from which the atomic description of the component is taken.

**[chem_comp]**

### _chem_comp.model_source (*text*)

The source of the coordinates for the model of the component.

Examples: 'CSD entry ABCDEF', 'built using Quanta/Charmm'.

**[chem_comp]**

### _chem_comp.mon_nstd_class (*text*)

A description of the class of a nonstandard monomer if the nonstandard monomer represents a modification of a standard monomer.

Examples: 'iodinated base', 'phosphorylated amino acid', 'brominated base', 'modified amino acid', 'glycosylated amino acid'.

**[chem_comp]**

### _chem_comp.mon_nstd_details (*text*)

A description of special details of a nonstandard monomer.

**[chem_comp]**

### _chem_comp.mon_nstd_flag (*ucode*)

'yes' indicates that this is a 'standard' monomer, 'no' indicates that it is 'nonstandard'. Nonstandard monomers should be described in more detail using the **_chem_comp.mon_nstd_parent**, **_chem_comp.mon_nstd_class** and **_chem_comp.mon_nstd_details** data items.

The data value must be one of the following:

| | |
|---|---|
| no | the monomer is nonstandard |
| n | abbreviation for 'no' |
| yes | the monomer is standard |
| y | abbreviation for 'yes' |

Where no value is given, the assumed value is 'no'. **[chem_comp]**

### _chem_comp.mon_nstd_parent (*code*)

The name of the parent monomer of the nonstandard monomer, if the nonstandard monomer represents a modification of a standard monomer.

Examples: 'tyrosine', 'cytosine'. **[chem_comp]**

### _chem_comp.mon_nstd_parent_comp_id

The identifier for the parent component of the nonstandard component. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

### _chem_comp.name (*line*)

The full name of the component.

Examples: 'alanine', 'valine', 'adenine', 'cytosine'. **[chem_comp]**

### _chem_comp.number_atoms_all (*int*)

The total number of atoms in the component.

The permitted range is $[1, \infty)$. **[chem_comp]**

### _chem_comp.number_atoms_nh (*int*)

The number of non-hydrogen atoms in the component.

The permitted range is $[1, \infty)$. **[chem_comp]**

### _chem_comp.one_letter_code (*uchar1*)

For standard polymer components, the one-letter code for the component. If there is not a standard one-letter code for this component, or if this is a non-polymer component, the one-letter code should be given as 'X'. This code may be preceded by a '+' character to indicate that the component is a modification of a standard component.

Examples: 'A' (alanine or adenine), 'B' (ambiguous asparagine/aspartic acid), 'R' (arginine), 'N' (asparagine), 'D' (aspartic acid), 'C' (cysteine or cystine or cytosine), 'Q' (glutamine), 'E' (glutamic acid), 'Z' (ambiguous glutamine/glutamic acid), 'G' (glycine or guanine), 'H' (histidine), 'I' (isoleucine), 'L' (leucine), 'K' (lysine), 'M' (methionine), 'F' (phenylalanine), 'P' (proline), 'S' (serine), 'T' (threonine or thymine), 'W' (tryptophan), 'Y' (tyrosine), 'V' (valine), 'U' (uracil), 'O' (water), 'X' (other). **[chem_comp]**

### _chem_comp.three_letter_code (*uchar3*)

For standard polymer components, the three-letter code for the component. If there is not a standard three-letter code for this component, or if this is a non-polymer component, the three-letter code should be given as 'UNK'. This code may be preceded by a '+' character to indicate that the component is a modification of a standard component.

Examples: 'ALA' (alanine), 'ARG' (arginine), 'ASN' (asparagine), 'ASP' (aspartic acid), 'ASX' (ambiguous asparagine/aspartic acid), 'CYS' (cysteine), 'GLN' (glutamine), 'GLU' (glutamic acid), 'GLY' (glycine), 'GLX' (ambiguous glutamine/glutamic acid), 'HIS' (histidine), 'ILE' (isoleucine), 'LEU' (leucine), 'LYS' (lysine), 'MET' (methionine), 'PHE' (phenylalanine), 'PRO' (proline), 'SER' (serine), 'THR' (threonine), 'TRP' (tryptophan), 'TRY' (tyrosine), 'VAL' (valine), '1MA' (1-methyladenosine), '5MC' (5-methylcytosine), 'OMC' (2′-*O*-methylcytodine), '1MG' (1-methylguanosine), '2MG' (N(2)-methylguanosine), 'M2G' (N(2)-dimethylguanosine), '7MG' (7-methylguanosine), 'OMG' (2′-*O*-methylguanosine), 'H2U' (dihydrouridine), '5MU' (ribosylthymidine), 'PSU' (pseudouridine), 'ACE' (acetic acid), 'FOR' (formic acid), 'HOH' (water), 'UNK' (other). **[chem_comp]**

* **_chem_comp.type** (*uline*)
For standard polymer components, the type of the monomer. Note that monomers that will form polymers are of three types: linking monomers, monomers with some type of N-terminal (or 5′) cap and monomers with some type of C-terminal (or 3′) cap.

*The following item(s) have an equivalent role in their respective categories:*

***_chem_comp_link.type_comp_1***,
***_chem_comp_link.type_comp_2***.

The data value must be one of the following:

```
'D-peptide linking'
'L-peptide linking'
'D-peptide NH3 amino terminus'
'L-peptide NH3 amino terminus'
'D-peptide COOH carboxy terminus'
'L-peptide COOH carboxy terminus'
'DNA linking'
'RNA linking'
'DNA OH 5 prime terminus'
'RNA OH 5 prime terminus'
'DNA OH 3 prime terminus'
'RNA OH 3 prime terminus'
'D-saccharide 1,4 and 1,4 linking'
'L-saccharide 1,4 and 1,4 linking'
'D-saccharide 1,4 and 1,6 linking'
'L-saccharide 1,4 and 1,6 linking'
L-saccharide
D-saccharide
saccharide
non-polymer
other
```
**[chem_comp]**

## CHEM_COMP_ANGLE

Data items in the CHEM_COMP_ANGLE category record details about angles in a chemical component. Angles are designated by three atoms, with the second atom forming the vertex of the angle. Target values may be specified as angles in degrees, as a distance between the first and third atoms, or both.

Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_angle.comp_id**
**_chem_comp_angle.atom_id_1**
**_chem_comp_angle.atom_id_2**
**_chem_comp_angle.atom_id_3**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_angle.comp_id
_chem_comp_angle.atom_id_1
_chem_comp_angle.atom_id_2
_chem_comp_angle.atom_id_3
_chem_comp_angle.value_angle
_chem_comp_angle.value_dist
  phe  N    CA   C    xxx.xx   x.xx
  phe  CA   C    O    xxx.xx   x.xx
  phe  CB   CA   C    xxx.xx   x.xx
  phe  CB   CA   N    xxx.xx   x.xx
  phe  CA   CB   CG   xxx.xx   x.xx
  phe  CB   CG   CD1  xxx.xx   x.xx
  phe  CB   CG   CD2  xxx.xx   x.xx
  phe  CD1  CG   CD2  xxx.xx   x.xx
  phe  CG   CD1  CE1  xxx.xx   x.xx
  phe  CD1  CE1  CZ   xxx.xx   x.xx
  phe  CE1  CZ   CE2  xxx.xx   x.xx
  phe  CZ   CE2  CD2  xxx.xx   x.xx
  phe  CG   CD2  CE2  xxx.xx   x.xx
  val  N    CA   C    xxx.xx   x.xx
  val  CA   C    O    xxx.xx   x.xx
  val  CB   CA   C    xxx.xx   x.xx
  val  CB   CA   N    xxx.xx   x.xx
  val  CA   CB   CG1  xxx.xx   x.xx
  val  CA   CB   CG2  xxx.xx   x.xx
  val  CG1  CB   CG2  xxx.xx   x.xx
```

* **_chem_comp_angle.atom_id_1**
The ID of the first of the three atoms that define the angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_angle.atom_id_2**
The ID of the second of the three atoms that define the angle. The second atom is taken to be the apex of the angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_angle.atom_id_3**
The ID of the third of the three atoms that define the angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_angle.comp_id**
This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

**_chem_comp_angle.value_angle** (*float, su*)
The value that should be taken as the target value for the angle associated with the specified atoms, expressed in degrees.

The permitted range is [0.0, 180.0].

Related item: **_chem_comp_angle.value_angle_esd** (associated esd).

**[chem_comp_angle]**

**_chem_comp_angle.value_angle_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_angle.value_angle**.

The permitted range is [0.0, 180.0].

Related item: **_chem_comp_angle.value_angle** (associated value).

**[chem_comp_angle]**

**_chem_comp_angle.value_dist** (*float, su*)
The value that should be taken as the target value for the angle associated with the specified atoms, expressed as the distance between the atoms specified by **_chem_comp_angle.atom_id_1** and **_chem_comp_angle.atom_id_3**.

The permitted range is $[0.0, \infty)$.

Related item: **_chem_comp_angle.value_dist_esd** (associated esd).

**[chem_comp_angle]**

**_chem_comp_angle.value_dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_angle.value_dist**.

The permitted range is $[0.0, \infty)$.

Related item: **_chem_comp_angle.value_dist** (associated value).

**[chem_comp_angle]**

## CHEM_COMP_ATOM

Data items in the CHEM_COMP_ATOM category record details about the atoms in a chemical component. Specifying the atomic coordinates for the components in this category is an alternative to specifying the structure of the component *via* bonds, angles, planes *etc.* in the appropriate CHEM_COMP subcategories.

Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_atom.comp_id**
**_chem_comp_atom.atom_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_atom.comp_id
_chem_comp_atom.atom_id
_chem_comp_atom.type_symbol
_chem_comp_atom.substruct_code
_chem_comp_atom.model_Cartn_x
_chem_comp_atom.model_Cartn_y
_chem_comp_atom.model_Cartn_z
  phe  N    N  main    1.20134   0.84658   0.00000
  phe  CA   C  main    0.00000   0.00000   0.00000
  phe  C    C  main   -1.25029   0.88107   0.00000
  phe  O    O  main   -2.18525   0.66029  -0.78409
  phe  CB   C  side    0.00662  -1.03603   1.11081
  phe  CG   C  side    0.03254  -0.49711   2.50951
  phe  CD1  C  side   -1.15813  -0.12084   3.13467
  phe  CE1  C  side   -1.15720   0.38038   4.42732
  phe  CZ   C  side    0.05385   0.51332   5.11032
  phe  CE2  C  side    1.26137   0.11613   4.50975
  phe  CD2  C  side    1.23668  -0.38351   3.20288
  val  N    N  main    1.20134   0.84658   0.00000
  val  CA   C  main    0.00000   0.00000   0.00000
  val  C    C  main   -1.25029   0.88107   0.00000
  val  O    O  main   -2.18525   0.66029  -0.78409
  val  CB   C  side    0.05260  -0.99339   1.17429
  val  CG1  C  side   -0.13288  -0.31545   2.52668
  val  CG2  C  side   -0.94265  -2.12930   0.99811
```

### _chem_comp_atom.alt_atom_id (*line*)

An alternative identifier for the atom. This data item would be used in cases where alternative nomenclatures exist for labelling atoms in a group.

**[chem_comp_atom]**

### *_chem_comp_atom.atom_id (*atcode*)

The value of **_chem_comp_atom.atom_id** must uniquely identify each atom in each monomer in the CHEM_COMP_ATOM list. The atom identifiers need not be unique over all atoms in the data block; they need only be unique for each atom in a component. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_site.label_atom_id***,
***_chem_comp_angle.atom_id_1***,
***_chem_comp_angle.atom_id_2***,
***_chem_comp_angle.atom_id_3***,
***_chem_comp_bond.atom_id_1***,
***_chem_comp_bond.atom_id_2***,
***_chem_comp_chir.atom_id***,
***_chem_comp_chir_atom.atom_id***,
***_chem_comp_plane_atom.atom_id***,
***_chem_comp_tor.atom_id_1***,
***_chem_comp_tor.atom_id_2***,
***_chem_comp_tor.atom_id_3***,
***_chem_comp_tor.atom_id_4***,
***_geom_angle.atom_site_label_atom_id_1***,
***_geom_angle.atom_site_label_atom_id_2***,
***_geom_angle.atom_site_label_atom_id_3***,
***_geom_bond.atom_site_label_atom_id_1***,
***_geom_bond.atom_site_label_atom_id_2***,
***_geom_contact.atom_site_label_atom_id_1***,
***_geom_contact.atom_site_label_atom_id_2***,
***_geom_hbond.atom_site_label_atom_id_A***,
***_geom_hbond.atom_site_label_atom_id_D***,
***_geom_hbond.atom_site_label_atom_id_H***,
***_geom_torsion.atom_site_label_atom_id_1***,
***_geom_torsion.atom_site_label_atom_id_2***,
***_geom_torsion.atom_site_label_atom_id_3***,
***_geom_torsion.atom_site_label_atom_id_4***,
***_struct_conn.ptnr1_label_atom_id***,
***_struct_conn.ptnr2_label_atom_id***,
***_struct_sheet_hbond.range_1_beg_label_atom_id***,
***_struct_sheet_hbond.range_1_end_label_atom_id***,
***_struct_sheet_hbond.range_2_beg_label_atom_id***,
***_struct_sheet_hbond.range_2_end_label_atom_id***,
***_struct_site_gen.label_atom_id***. **[chem_comp_atom]**

### _chem_comp_atom.charge (*int*)

The net integer charge assigned to this atom. This is the formal charge assignment normally found in chemical diagrams.

The permitted range is $[-8, 8]$. Where no value is given, the assumed value is '0'.

Examples: '1' (for an ammonium nitrogen), '-1' (for a chloride ion).

**[chem_comp_atom]**

### *_chem_comp_atom.comp_id

This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

### _chem_comp_atom.model_Cartn_x (*float, su*)

The *x* component of the coordinates for this atom in this component specified as orthogonal ångströms. The choice of reference axis frame for the coordinates is arbitrary. The set of coordinates input for the entity here is intended to correspond to the atomic model used to generate restraints for structure refinement, not to atom sites in the ATOM_SITE list.

Related item: **_chem_comp_atom.model_Cartn_x_esd** (associated esd).

**[chem_comp_atom]**

### _chem_comp_atom.model_Cartn_x_esd (*float*)

The standard uncertainty (estimated standard deviation) of **_chem_comp_atom.model_Cartn_x**.

Related item: **_chem_comp_atom.model_Cartn_x** (associated value).

**[chem_comp_atom]**

### _chem_comp_atom.model_Cartn_y (*float, su*)

The *y* component of the coordinates for this atom in this component specified as orthogonal ångströms. The choice of reference axis frame for the coordinates is arbitrary. The set of coordinates input for the entity here is intended to correspond to the atomic model used to generate restraints for structure refinement, not to atom sites in the ATOM_SITE list.

Related item: **_chem_comp_atom.model_Cartn_y_esd** (associated esd).

**[chem_comp_atom]**

### _chem_comp_atom.model_Cartn_y_esd (*float*)

The standard uncertainty (estimated standard deviation) of **_chem_comp_atom.model_Cartn_y**.

Related item: **_chem_comp_atom.model_Cartn_y** (associated value).

**[chem_comp_atom]**

**_chem_comp_atom.model_Cartn_z** (*float, su*)
The $z$ component of the coordinates for this atom in this component specified as orthogonal ångströms. The choice of reference axis frame for the coordinates is arbitrary. The set of coordinates input for the entity here is intended to correspond to the atomic model used to generate restraints for structure refinement, not to atom sites in the ATOM_SITE list.
Related item: **_chem_comp_atom.model_Cartn_z_esd** (associated esd).
**[chem_comp_atom]**

**_chem_comp_atom.model_Cartn_z_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_atom.model_Cartn_z**.
Related item: **_chem_comp_atom.model_Cartn_z** (associated value).
**[chem_comp_atom]**

**_chem_comp_atom.partial_charge** (*float*)
The partial charge assigned to this atom.
**[chem_comp_atom]**

**_chem_comp_atom.substruct_code** (*ucode*)
This data item assigns the atom to a substructure of the component, if appropriate.
The data value must be one of the following:

| | |
|---|---|
| main | main chain of an amino acid |
| side | side chain of an amino acid |
| base | base of a nucleic acid |
| phos | phosphate of a nucleic acid |
| sugar | sugar of a nucleic acid |
| none | not appropriate for this monomer |

**[chem_comp_atom]**

***_chem_comp_atom.type_symbol**
This data item is a pointer to **_atom_type.symbol** in the ATOM_TYPE category.

## CHEM_COMP_BOND

Data items in the CHEM_COMP_BOND category record details about the bonds between atoms in a chemical component. Target values may be specified as bond orders, as a distance between the two atoms, or both.
Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_bond.comp_id**
**_chem_comp_bond.atom_id_1**
**_chem_comp_bond.atom_id_2**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_bond.comp_id
_chem_comp_bond.atom_id_1
_chem_comp_bond.atom_id_2
_chem_comp_bond.value_order
  phe  N    CA   sing
  phe  CA   C    sing
  phe  C    O    doub
  phe  CB   CA   sing
  phe  CB   CG   sing
  phe  CG   CD1  arom
  phe  CD1  CE1  arom
  phe  CE1  CZ   arom
  phe  CZ   CE2  arom
  phe  CE2  CD2  arom
  phe  CD2  CG   arom
  val  N    CA   sing
  val  CA   C    sing
  val  C    O    doub
  val  CB   CA   sing
  val  CB   CG1  sing
  val  CB   CG2  sing
```

***_chem_comp_bond.atom_id_1**
The ID of the first of the two atoms that define the bond. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_chem_comp_bond.atom_id_2**
The ID of the second of the two atoms that define the bond. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_chem_comp_bond.comp_id**
This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

**_chem_comp_bond.value_dist** (*float, su*)
The value that should be taken as the target for the chemical bond associated with the specified atoms, expressed as a distance.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_comp_bond.value_dist_esd** (associated esd).
**[chem_comp_bond]**

**_chem_comp_bond.value_dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_bond.value_dist**.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_comp_bond.value_dist** (associated value).
**[chem_comp_bond]**

**_chem_comp_bond.value_order** (*ucode*)
The value that should be taken as the target for the chemical bond associated with the specified atoms, expressed as a bond order.
The data value must be one of the following:

| | |
|---|---|
| sing | single bond |
| doub | double bond |
| trip | triple bond |
| quad | quadruple bond |
| arom | aromatic bond |
| poly | polymeric bond |
| delo | delocalized double bond |
| pi | $\pi$ bond |

Where no value is given, the assumed value is 'sing'. **[chem_comp_bond]**

## CHEM_COMP_CHIR

Data items in the CHEM_COMP_CHIR category provide details about the chiral centres in a chemical component. The atoms bonded to the chiral atom are specified in the CHEM_COMP_CHIR_ATOM category.
Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_chir.comp_id**
**_chem_comp_chir.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_chir.comp_id
_chem_comp_chir.id
_chem_comp_chir.atom_id
  phe  phe1  CA
  val  val1  CA
# - - - - data truncated for brevity - - - -
```

**_chem_comp_chir.atom_config** (*ucode*)
The chiral configuration of the atom that is a chiral centre.
The data value must be one of the following:

| | |
|---|---|
| R | absolute configuration *R* |
| S | absolute configuration *S* |

[chem_comp_chir]

*_chem_comp_chir.atom_id
The ID of the atom that is a chiral centre. This data item is a pointer to _chem_comp_atom.atom_id in the CHEM_COMP_ATOM category.

*_chem_comp_chir.comp_id
This data item is a pointer to _chem_comp.id in the CHEM_COMP category.

*_chem_comp_chir.id (*code*)
The value of _chem_comp_chir.id must uniquely identify a record in the CHEM_COMP_CHIR list.
*The following item(s) have an equivalent role in their respective categories:*
*_chem_comp_chir_atom.chir_id.* [chem_comp_chir]

_chem_comp_chir.number_atoms_all (*int*)
The total number of atoms bonded to the atom specified by _chem_comp_chir.atom_id.
[chem_comp_chir]

_chem_comp_chir.number_atoms_nh (*int*)
The number of non-hydrogen atoms bonded to the atom specified by _chem_comp_chir.atom_id.
[chem_comp_chir]

_chem_comp_chir.volume_flag (*ucode*)
A flag to indicate whether a chiral volume should match the standard value in both magnitude and sign, or in magnitude only.
The data value must be one of the following:

| | |
|---|---|
| sign | match magnitude and sign |
| nosign | match magnitude only |

[chem_comp_chir]

_chem_comp_chir.volume_three (*float, su*)
The chiral volume, $V_c$, for chiral centres that involve a chiral atom bonded to three non-hydrogen atoms and one hydrogen atom.

$$V_c = \mathbf{V}_1 \cdot (\mathbf{V}_2 \times \mathbf{V}_3),$$

where $\mathbf{V}_1$ = the vector distance from the atom specified by _chem_comp_chir.atom_id to the first atom in the CHEM_COMP_CHIR_ATOM list, $\mathbf{V}_2$ = the vector distance from the atom specified by _chem_comp_chir.atom_id to the second atom in the CHEM_COMP_CHIR_ATOM list, $\mathbf{V}_3$ = the vector distance from the atom specified by _chem_comp_chir.atom_id to the third atom in the CHEM_COMP_CHIR_ATOM list, $\cdot$ = the vector dot product and $\times$ = the vector cross product.
Related item: _chem_comp_chir.volume_three_esd (associated esd).
[chem_comp_chir]

_chem_comp_chir.volume_three_esd (*float*)
The standard uncertainty (estimated standard deviation) of _chem_comp_chir.volume_three.
Related item: _chem_comp_chir.volume_three (associated value).
[chem_comp_chir]

## CHEM_COMP_CHIR_ATOM

Data items in the CHEM_COMP_CHIR_ATOM category enumerate the atoms bonded to a chiral atom within a chemical component.
Category group(s): inclusive_group
chem_comp_group
Category key(s): _chem_comp_chir_atom.chir_id
_chem_comp_chir_atom.atom_id
_chem_comp_chir_atom.comp_id

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_chir_atom.comp_id
_chem_comp_chir_atom.chir_id
_chem_comp_chir_atom.atom_id
  phe  1  N
  phe  1  C
  phe  1  CB
  val  1  N
  val  1  C
  val  1  CB
   # - - - - data truncated for brevity - - - -
```

*_chem_comp_chir_atom.atom_id
The ID of an atom bonded to the chiral atom.
This data item is a pointer to _chem_comp_atom.atom_id in the CHEM_COMP_ATOM category.

*_chem_comp_chir_atom.chir_id
This data item is a pointer to _chem_comp_chir.id in the CHEM_COMP_CHIR category.

*_chem_comp_chir_atom.comp_id
This data item is a pointer to _chem_comp.id in the CHEM_COMP category.

_chem_comp_chir_atom.dev (*float*)
The standard uncertainty (estimated standard deviation) of the position of this atom from the plane defined by all of the atoms in the plane.
[chem_comp_chir_atom]

## CHEM_COMP_LINK

Data items in the CHEM_COMP_LINK category give details about the links between chemical components.
Category group(s): inclusive_group
chem_link_group
Category key(s): _chem_comp_link.link_id

_chem_comp_link.details (*text*)
A description of special aspects of a link between chemical components in the structure.
[chem_comp_link]

*_chem_comp_link.link_id
This data item is a pointer to _chem_link.id in the CHEM_LINK category.

*_chem_comp_link.type_comp_1
The type of the first of the two components joined by the link. This data item is a pointer to _chem_comp.type in the CHEM_COMP category.

* **_chem_comp_link.type_comp_2**
The type of the second of the two components joined by the link. This data item is a pointer to **_chem_comp.type** in the CHEM_COMP category.

### CHEM_COMP_PLANE

Data items in the CHEM_COMP_PLANE category provide identifiers for the planes in a chemical component. The atoms in the plane are specified in the CHEM_COMP_PLANE_ATOM category.

Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_plane.comp_id**
**_chem_comp_plane.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_plane.comp_id
_chem_comp_plane.id
  phe  phe1
```

* **_chem_comp_plane.comp_id**
This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

* **_chem_comp_plane.id** (*code*)
The value of **_chem_comp_plane.id** must uniquely identify a record in the CHEM_COMP_PLANE list.

*The following item(s) have an equivalent role in their respective categories:*

***_chem_comp_plane_atom.plane_id***. **[chem_comp_plane]**

**_chem_comp_plane.number_atoms_all** (*int*)
The total number of atoms in the plane.

**[chem_comp_plane]**

**_chem_comp_plane.number_atoms_nh** (*int*)
The number of non-hydrogen atoms in the plane.

**[chem_comp_plane]**

### CHEM_COMP_PLANE_ATOM

Data items in the CHEM_COMP_PLANE_ATOM category enumerate the atoms in a plane within a chemical component.

Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_plane_atom.plane_id**
**_chem_comp_plane_atom.atom_id**
**_chem_comp_plane_atom.comp_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_plane_atom.plane_id
_chem_comp_plane_atom.comp_id
_chem_comp_plane_atom.atom_id
  phe1  phe  CB
  phe1  phe  CG
  phe1  phe  CD1
  phe1  phe  CE1
  phe1  phe  CZ
  phe1  phe  CE2
  phe1  phe  CD2
```

* **_chem_comp_plane_atom.atom_id**
The ID of an atom involved in the plane. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_plane_atom.comp_id**
This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

**_chem_comp_plane_atom.dist_esd** (*float*)
This data item is the standard deviation of the out-of-plane distance for this atom.

* **_chem_comp_plane_atom.plane_id**
This data item is a pointer to **_chem_comp_plane.id** in the CHEM_COMP_PLANE category.

### CHEM_COMP_TOR

Data items in the CHEM_COMP_TOR category record details about the torsion angles in a chemical component. As torsion angles can have more than one target value, the target values are specified in the CHEM_COMP_TOR_VALUE category.

Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_tor.comp_id**
**_chem_comp_tor.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_tor.comp_id
_chem_comp_tor.id
_chem_comp_tor.atom_id_1
_chem_comp_tor.atom_id_2
_chem_comp_tor.atom_id_3
_chem_comp_tor.atom_id_4
  phe  phe_chi1   N    CA   CB   CG
  phe  phe_chi2   CA   CB   CG   CD1
  phe  phe_ring1  CB   CG   CD1  CE1
  phe  phe_ring2  CB   CG   CD2  CE2
  phe  phe_ring3  CG   CD1  CE1  CZ
  phe  phe_ring4  CD1  CE1  CZ   CE2
  phe  phe_ring5  CE1  CZ   CE2  CD2
```

* **_chem_comp_tor.atom_id_1**
The ID of the first of the four atoms that define the torsion angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_tor.atom_id_2**
The ID of the second of the four atoms that define the torsion angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_tor.atom_id_3**
The ID of the third of the four atoms that define the torsion angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_tor.atom_id_4**
The ID of the fourth of the four atoms that define the torsion angle. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

* **_chem_comp_tor.comp_id**
This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

***_chem_comp_tor.id** (*code*)
The value of **_chem_comp_tor.id** must uniquely identify a record in the CHEM_COMP_TOR list.
*The following item(s) have an equivalent role in their respective categories:*
***_chem_comp_tor_value.tor_id***. **[chem_comp_tor]**

## CHEM_COMP_TOR_VALUE

Data items in the CHEM_COMP_TOR_VALUE category record details about the target values for the torsion angles enumerated in the CHEM_COMP_TOR list. Target values may be specified as angles in degrees, as a distance between the first and fourth atoms, or both.
Category group(s): **inclusive_group**
**chem_comp_group**
Category key(s): **_chem_comp_tor_value.tor_id**
**_chem_comp_tor_value.comp_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_chem_comp_tor_value.tor_id
_chem_comp_tor_value.comp_id
_chem_comp_tor_value.angle
_chem_comp_tor_value.dist
  phe_chi1   phe  -60.0  2.88
  phe_chi1   phe  180.0  3.72
  phe_chi1   phe   60.0  2.88
  phe_chi2   phe   90.0  3.34
  phe_chi2   phe  -90.0  3.34
  phe_ring1  phe  180.0  3.75
  phe_ring2  phe  180.0  3.75
  phe_ring3  phe    0.0  2.80
  phe_ring4  phe    0.0  2.80
  phe_ring5  phe    0.0  2.80
```

***_chem_comp_tor_value.angle** (*float, su*)
A value that should be taken as a potential target value for the torsion angle associated with the specified atoms, expressed in degrees.
The permitted range is $[-180.0, 180.0]$.
Related item: **_chem_comp_tor_value.angle_esd** (associated esd).
**[chem_comp_tor_value]**

***_chem_comp_tor_value.angle_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_tor_value.angle**.
The permitted range is $[-180.0, 180.0]$.
Related item: **_chem_comp_tor_value.angle** (associated value).
**[chem_comp_tor_value]**

***_chem_comp_tor_value.comp_id**
This data item is a pointer to **_chem_comp_atom.comp_id** in the CHEM_COMP_ATOM category.

**_chem_comp_tor_value.dist** (*float, su*)
A value that should be taken as a potential target value for the torsion angle associated with the specified atoms, expressed as the distance between the atoms specified by **_chem_comp_tor.atom_id_1** and **_chem_comp_tor.atom_id_4** in the referenced record in the CHEM_COMP_TOR list. Note that the torsion angle cannot be fully specified by a distance (for instance, a torsion angle of $-60°$ will yield the same distance as a $60°$ angle). However, the distance specification can be useful for refinement in situations in which the angle is already close to the desired value.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_comp_tor_value.dist_esd** (associated esd).
**[chem_comp_tor_value]**

**_chem_comp_tor_value.dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_tor_value.dist**.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_comp_tor_value.dist** (associated value).
**[chem_comp_tor_value]**

***_chem_comp_tor_value.tor_id**
This data item is a pointer to **_chem_comp_tor.id** in the CHEM_COMP_TOR category.

## CHEM_LINK

Data items in the CHEM_LINK category give details about the links between chemical components.
Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link.id**

**_chem_link.details** (*text*)
A description of special aspects of a link between chemical components in the structure.
**[chem_link]**

***_chem_link.id** (*code*)
The value of **_chem_link.id** must uniquely identify each item in the CHEM_LINK list.
*The following item(s) have an equivalent role in their respective categories:*
***_chem_link_angle.link_id***,
***_chem_link_bond.link_id***,
***_chem_link_chir.link_id***,
***_chem_link_plane.link_id***,
***_chem_link_tor.link_id***,
***_chem_comp_link.link_id***,
***_entity_link.link_id***.
Examples: ‘peptide’, ‘oligosaccharide 1,4’, ‘DNA’. **[chem_link]**

## CHEM_LINK_ANGLE

Data items in the CHEM_LINK_ANGLE category record details about angles in a link between chemical components.
Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_angle.link_id**
**_chem_link_angle.atom_id_1**
**_chem_link_angle.atom_id_2**
**_chem_link_angle.atom_id_3**

*Example 1 – Engh & Huber parameters [Acta Cryst. (1991), A**47**, 392–400] as interpreted by J. P. Priestle (1995). Consistent Stereochemical Dictionaries for Refinement and Model Building. CCP4 Daresbury Study Weekend, DL-CONF-95-001, ISSN 1358-6254. Warrington: Daresbury Laboratory.*

```
loop_
_chem_link_angle.link_id
_chem_link_angle.value_angle
_chem_link_angle.value_angle_esd
_chem_link_angle.atom_id_1
_chem_link_angle.atom_1_comp_id
_chem_link_angle.atom_id_2
_chem_link_angle.atom_2_comp_id
_chem_link_angle.atom_id_3
_chem_link_angle.atom_3_comp_id
 PEPTIDE  111.2  2.8  N  1  CA 1  C  1
 PEPTIDE  120.8  1.7  CA 1  C  1  O  1
 PEPTIDE  116.2  2.0  CA 1  C  1  N  2
 PEPTIDE  123.0  1.6  O  1  C  1  N  2
 PEPTIDE  121.7  1.8  C  1  N  2  CA 2
```

**_chem_link_angle.atom_1_comp_id** (*ucode*)
This data item indicates whether atom 1 is found in the first or the second of the two components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_angle]**

**_chem_link_angle.atom_2_comp_id** (*ucode*)
This data item indicates whether atom 2 is found in the first or the second of the two components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_angle]**

**_chem_link_angle.atom_3_comp_id** (*ucode*)
This data item indicates whether atom 3 is found in the first or the second of the two components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_angle]**

***_chem_link_angle.atom_id_1** (*code*)
The ID of the first of the three atoms that define the angle. An atom with this ID must exist in the component of the type specified by **_chem_comp_link.type_comp_1** (or **_chem_comp_link.type_comp_2**, where the appropriate data item is indicated by the value of **_chem_comp_angle.atom_1_comp_id**).
**[chem_link_angle]**

***_chem_link_angle.atom_id_2** (*code*)
The ID of the second of the three atoms that define the angle. The second atom is taken to be the apex of the angle. An atom with this ID must exist in the component of the type specified by **_chem_comp_link.type_comp_1** (or **_chem_comp_link.type_comp_2**, where the appropriate data item is indicated by the value of **_chem_comp_angle.atom_2_comp_id**).
**[chem_link_angle]**

***_chem_link_angle.atom_id_3** (*code*)
The ID of the third of the three atoms that define the angle. An atom with this ID must exist in the component of the type specified by **_chem_comp_link.type_comp_1** (or **_chem_comp_link.type_comp_2**, where the appropriate data item is indicated by the value of **_chem_comp_angle.atom_3_comp_id**).
**[chem_link_angle]**

***_chem_link_angle.link_id**
This data item is a pointer to **_chem_link.id** in the CHEM_LINK category.

**_chem_link_angle.value_angle** (*float, su*)
The value that should be taken as the target value for the angle associated with the specified atoms, expressed in degrees.
The permitted range is [0.0, 180.0].
Related item: **_chem_link_angle.value_angle_esd** (associated esd).
**[chem_link_angle]**

**_chem_link_angle.value_angle_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_link_angle.value_angle**.
The permitted range is [0.0, 180.0].
Related item: **_chem_link_angle.value_angle** (associated value).
**[chem_link_angle]**

**_chem_link_angle.value_dist** (*float, su*)
The value that should be taken as the target value for the angle associated with the specified atoms, expressed as the distance between the atoms specified by **_chem_comp_angle.atom_id_1** and **_chem_comp_angle.atom_id_3**.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_link_angle.value_dist_esd** (associated esd).
**[chem_link_angle]**

**_chem_link_angle.value_dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_comp_angle.value_dist**.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_link_angle.value_dist** (associated value).
**[chem_link_angle]**

## CHEM_LINK_BOND

Data items in the CHEM_LINK_BOND category record details about bonds in a link between components in the chemical structure.

Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_bond.link_id**
**_chem_link_bond.atom_id_1**
**_chem_link_bond.atom_id_2**

*Example 1 – Engh & Huber parameters [Acta Cryst. (1991), A**47**, 392–400] as interpreted by J. P. Priestle (1995). Consistent Stereochemical Dictionaries for Refinement and Model Building. CCP4 Daresbury Study Weekend, DL-CONF-95-001, ISSN 1358-6254. Warrington: Daresbury Laboratory.*

```
loop_
_chem_link_bond.link_id
_chem_link_bond.value_dist
_chem_link_bond.value_dist_esd
_chem_link_bond.atom_id_1
_chem_link_bond.atom_1_comp_id
_chem_link_bond.atom_id_2
_chem_link_bond.atom_2_comp_id
 PEPTIDE  1.458  0.019  N  1  CA 1
 PEPTIDE  1.525  0.021  CA 1  C  1
 PEPTIDE  1.329  0.014  C  1  N  2
 PEPTIDE  1.231  0.020  C  1  O  1
```

**_chem_link_bond.atom_1_comp_id** (*ucode*)
This data item indicates whether atom 1 is found in the first or the second of the two components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_bond]**

**_chem_link_bond.atom_2_comp_id** (*ucode*)
This data item indicates whether atom 2 is found in the first or the second of the two chemical components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_bond]**

* **_chem_link_bond.atom_id_1** (*code*)
The ID of the first of the two atoms that define the bond. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.
**[chem_link_bond]**

* **_chem_link_bond.atom_id_2** (*code*)
The ID of the second of the two atoms that define the bond. As this data item does not point to a specific atom in a specific component, it is not a child in the linkage sense.
**[chem_link_bond]**

* **_chem_link_bond.link_id**
This data item is a pointer to **_chem_link.id** in the CHEM_LINK category.

**_chem_link_bond.value_dist** (*float, su*)
The value that should be taken as the target for the chemical bond associated with the specified atoms, expressed as a distance.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_link_bond.value_dist_esd** (associated esd).
**[chem_link_bond]**

**_chem_link_bond.value_dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_link_bond.value_dist**.
The permitted range is $[0.0, \infty)$.
Related item: **_chem_link_bond.value_dist** (associated value).
**[chem_link_bond]**

**_chem_link_bond.value_order** (*ucode*)
The value that should be taken as the target for the chemical bond associated with the specified atoms, expressed as a bond order.
The data value must be one of the following:

| | |
|---|---|
| sing | single bond |
| doub | double bond |
| trip | triple bond |
| quad | quadruple bond |
| arom | aromatic bond |
| poly | polymeric bond |
| delo | delocalized double bond |
| pi | $\pi$ bond |

Where no value is given, the assumed value is '**sing**'. **[chem_link_bond]**

## CHEM_LINK_CHIR

Data items in the CHEM_LINK_CHIR category provide details about the chiral centres in a link between two chemical components. The atoms bonded to the chiral atom are specified in the CHEM_LINK_CHIR_ATOM category.
Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_chir.link_id**
**_chem_link_chir.id**

**_chem_link_chir.atom_comp_id** (*ucode*)
This data item indicates whether the chiral atom is found in the first or the second of the two components connected by the link.
The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_chir]**

**_chem_link_chir.atom_config** (*ucode*)
The chiral configuration of the atom that is a chiral centre.
The data value must be one of the following:

| | |
|---|---|
| R | absolute configuration *R* |
| S | absolute configuration *S* |

**[chem_link_chir]**

* **_chem_link_chir.atom_id** (*code*)
The ID of the atom that is a chiral centre. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

* **_chem_link_chir.id** (*code*)
The value of **_chem_link_chir.id** must uniquely identify a record in the CHEM_LINK_CHIR list.
*The following item(s) have an equivalent role in their respective categories:*
***_chem_link_chir_atom.chir_id***. **[chem_link_chir]**

* **_chem_link_chir.link_id**
This data item is a pointer to **_chem_link.id** in the CHEM_LINK category.

**_chem_link_chir.number_atoms_all** (*int*)
The total number of atoms bonded to the atom specified by **_chem_link_chir.atom_id**.
**[chem_link_chir]**

**_chem_link_chir.number_atoms_nh** (*int*)
The number of non-hydrogen atoms bonded to the atom specified by **_chem_link_chir.atom_id**.
**[chem_link_chir]**

**_chem_link_chir.volume_flag** (*ucode*)
A flag to indicate whether a chiral volume should match the standard value in both magnitude and sign, or in magnitude only.
The data value must be one of the following:

| | |
|---|---|
| sign | match magnitude and sign |
| nosign | match magnitude only |

**[chem_link_chir]**

**_chem_link_chir.volume_three** (*float, su*)
The chiral volume, $V_c$, for chiral centres that involve a chiral atom bonded to three non-hydrogen atoms and one hydrogen atom.

$$V_c = \mathbf{V}_1 \cdot (\mathbf{V}_2 \times \mathbf{V}_3),$$

where $\mathbf{V}_1$ = the vector distance from the atom specified by **_chem_link_chir.atom_id** to the first atom in the CHEM_LINK_CHIR_ATOM list, $\mathbf{V}_2$ = the vector distance from the atom specified by **_chem_link_chir.atom_id** to the second atom in the CHEM_LINK_CHIR_ATOM list, $\mathbf{V}_3$ = the vector distance from the atom specified by **_chem_link_chir.atom_id** to the third atom in the CHEM_LINK_CHIR_ATOM list, $\cdot$ = the vector dot product and $\times$ = the vector cross product.
Related item: **_chem_link_chir.volume_three_esd** (associated esd).
**[chem_link_chir]**

**_chem_link_chir.volume_three_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_chem_link_chir.volume_three**.
Related item: **_chem_link_chir.volume_three** (associated value).
**[chem_link_chir]**

## CHEM_LINK_CHIR_ATOM

Data items in the CHEM_LINK_CHIR_ATOM category enumerate the atoms bonded to a chiral atom in a link between two chemical components.

Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_chir_atom.chir_id**
**_chem_link_chir_atom.atom_id**

**_chem_link_chir_atom.atom_comp_id** (*ucode*)
This data item indicates whether the atom bonded to a chiral atom is found in the first or the second of the two components connected by the link.

The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_chir_atom]**

***_chem_link_chir_atom.atom_id** (*code*)
The ID of an atom bonded to the chiral atom. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

***_chem_link_chir_atom.chir_id**
This data item is a pointer to **_chem_link_chir.id** in the CHEM_LINK_CHIR category.

**_chem_link_chir_atom.dev** (*float*)
The standard uncertainty (estimated standard deviation) of the position of this atom from the plane defined by all of the atoms in the plane.

**[chem_link_chir_atom]**

## CHEM_LINK_PLANE

Data items in the CHEM_LINK_PLANE category provide identifiers for the planes in a link between two chemical components. The atoms in the plane are specified in the CHEM_LINK_PLANE_ATOM category.

Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_plane.link_id**
**_chem_link_plane.id**

***_chem_link_plane.id** (*code*)
The value of **_chem_link_plane.id** must uniquely identify a record in the CHEM_LINK_PLANE list.

*The following item(s) have an equivalent role in their respective categories:*
***_chem_link_plane_atom.plane_id***. **[chem_link_plane]**

***_chem_link_plane.link_id**
This data item is a pointer to **_chem_link.id** in the CHEM_LINK category.

**_chem_link_plane.number_atoms_all** (*int*)
The total number of atoms in the plane.

**[chem_link_plane]**

**_chem_link_plane.number_atoms_nh** (*int*)
The number of non-hydrogen atoms in the plane.

**[chem_link_plane]**

## CHEM_LINK_PLANE_ATOM

Data items in the CHEM_LINK_PLANE_ATOM category enumerate the atoms in a plane in a link between two chemical components.

Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_plane_atom.plane_id**
**_chem_link_plane_atom.atom_id**

**_chem_link_plane_atom.atom_comp_id** (*ucode*)
This data item indicates whether the atom in a plane is found in the first or the second of the two components connected by the link.

The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_plane_atom]**

***_chem_link_plane_atom.atom_id** (*code*)
The ID of an atom involved in the plane. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

***_chem_link_plane_atom.plane_id**
This data item is a pointer to **_chem_link_plane.id** in the CHEM_LINK_PLANE category.

## CHEM_LINK_TOR

Data items in the CHEM_LINK_TOR category record details about the torsion angles in a link between two chemical components. As torsion angles can have more than one target value, the target values are specified in the CHEM_LINK_TOR_VALUE category.

Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_chem_link_tor.link_id**
**_chem_link_tor.id**

**_chem_link_tor.atom_1_comp_id** (*ucode*)
This data item indicates whether atom 1 is found in the first or the second of the two components connected by the link.

The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_tor]**

**_chem_link_tor.atom_2_comp_id** (*ucode*)
This data item indicates whether atom 2 is found in the first or the second of the two components connected by the link.

The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_tor]**

**_chem_link_tor.atom_3_comp_id** (*ucode*)
This data item indicates whether atom 3 is found in the first or the second of the two components connected by the link.

The data value must be one of the following:

| | |
|---|---|
| 1 | the atom is in component 1 |
| 2 | the atom is in component 2 |

**[chem_link_tor]**

**_chem_link_tor.atom_4_comp_id** (*ucode*)
This data item indicates whether atom 4 is found in the first or the second of the two components connected by the link.
The data value must be one of the following:
1 the atom is in component 1
2 the atom is in component 2
[chem_link_tor]

*_chem_link_tor.atom_id_1 (*code*)
The ID of the first of the four atoms that define the torsion angle. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

*_chem_link_tor.atom_id_2 (*code*)
The ID of the second of the four atoms that define the torsion angle. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

*_chem_link_tor.atom_id_3 (*code*)
The ID of the third of the four atoms that define the torsion angle. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

*_chem_link_tor.atom_id_4 (*code*)
The ID of the fourth of the four atoms that define the torsion angle. As this data item does not point to a specific atom in a specific chemical component, it is not a child in the linkage sense.

*_chem_link_tor.id (*code*)
The value of _chem_link_tor.id must uniquely identify a record in the CHEM_LINK_TOR list.
*The following item(s) have an equivalent role in their respective categories:*
*_chem_link_tor_value.tor_id*. [chem_link_tor]

*_chem_link_tor.link_id
This data item is a pointer to _chem_link.id in the CHEM_LINK category.

## CHEM_LINK_TOR_VALUE

Data items in the CHEM_LINK_TOR_VALUE category record details about the target values for the torsion angles enumerated in the CHEM_LINK_TOR list. Target values may be specified as angles in degrees, as a distance between the first and fourth atoms, or both.
Category group(s): inclusive_group
chem_link_group
Category key(s): _chem_link_tor_value.tor_id

*_chem_link_tor_value.angle (*float, su*)
A value that should be taken as a potential target value for the torsion angle associated with the specified atoms, expressed in degrees.
The permitted range is $[-180.0, 180.0]$.
Related item: _chem_link_tor_value.angle_esd (associated esd).
[chem_link_tor_value]

*_chem_link_tor_value.angle_esd (*float*)
The standard uncertainty (estimated standard deviation) of _chem_link_tor_value.angle.
The permitted range is $[-180.0, 180.0]$.
Related item: _chem_link_tor_value.angle (associated value).
[chem_link_tor_value]

_chem_link_tor_value.dist (*float, su*)
A value that should be taken as a potential target value for the torsion angle associated with the specified atoms, expressed as the distance between the atoms specified by _chem_link_tor.atom_id_1 and _chem_link_tor.atom_id_4 in the referenced record in the CHEM_LINK_TOR list. Note that the torsion angle cannot be fully specified by a distance (for instance, a torsion angle of $-60°$ will yield the same distance as a $60°$ angle). However, the distance specification can be useful for refinement in situations in which the angle is already close to the desired value.
The permitted range is $[0.0, \infty)$.
Related item: _chem_link_tor_value.dist_esd (associated esd).
[chem_link_tor_value]

_chem_link_tor_value.dist_esd (*float*)
The standard uncertainty (estimated standard deviation) of _chem_link_tor_value.dist.
The permitted range is $[0.0, \infty)$.
Related item: _chem_link_tor_value.dist (associated value).
[chem_link_tor_value]

*_chem_link_tor_value.tor_id
This data item is a pointer to _chem_link_tor.id in the CHEM_LINK_TOR category.

## CHEMICAL

Data items in the CHEMICAL category would not in general be used in a macromolecular CIF. See instead the ENTITY data items. Data items in the CHEMICAL category record details about the composition and chemical properties of the compounds. The formula data items must agree with those that specify the density, unit-cell and $Z$ values.
Category group(s): inclusive_group
chemical_group
Category key(s): _chemical.entry_id

*Example 1 – based on data set 9597gaus of Alyea, Ferguson & Kannan [Acta Cryst. (1996), **C52**, 765–767].*

```
_chemical.entry_id       '9597gaus'
_chemical.name_systematic
  trans-bis(tricyclohexylphosphine)tetracarbonylmolybdenum(0)
```

_chemical.absolute_configuration (*code*)
*_chemical_absolute_configuration* (*cif_core.dic 2.3*)
Necessary conditions for the assignment of _chemical.absolute_configuration are given by H. D. Flack and G. Bernardinelli (1999, 2000).

References: Flack, H. D. & Bernardinelli, G. (1999). *Acta Cryst.* A**55**, 908–915. Flack, H. D. & Bernardinelli, G. (2000). *J. Appl. Cryst.* **33**, 1143–1148.
The data value must be one of the following:
rm Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration.
ad Absolute configuration established by anomalous-dispersion effects in diffraction measurements on the crystal.
rmad Absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration and confirmed by anomalous-dispersion effects in diffraction measurements on the crystal.
syn Absolute configuration has not been established by anomalous-dispersion effects in diffraction measurements on the crystal. The enantiomer has been assigned by reference to an unchanging chiral centre in the synthetic procedure.

`unk` Absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous-dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made.

`.` Inapplicable.

**[chemical]**

### _chemical.compound_source (*text*)

***_chemical_compound_source*** (*cif_core.dic 2.0.1*)

Description of the source of the compound under study, or of the parent molecule if a simple derivative is studied. This includes the place of discovery for minerals or the actual source of a natural product.

Examples: 'From Norilsk (USSR)',
'Extracted from the bark of Cinchona Naturalis'. **[chemical]**

### *_chemical.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### _chemical.melting_point (*float*)

***_chemical_melting_point*** (*cif_core.dic 2.0.1*)

The temperature in kelvins at which the crystalline solid changes to a liquid.

The permitted range is $[0.0, \infty)$. **[chemical]**

### _chemical.melting_point_gt (*float*)

***_chemical_melting_point_gt*** (*cif_core.dic 2.3*)

A temperature in kelvins above which the melting point (the temperature at which the crystalline solid changes to a liquid) lies. **_chemical.melting_point_gt** and **_chemical.melting_point_lt** allow a range of temperatures to be given. **_chemical.melting_point** should always be used in preference to these two items whenever possible.

The permitted range is $[0.0, \infty)$.

Related item: **_chemical.melting_point** (alternate). **[chemical]**

### _chemical.melting_point_lt (*float*)

***_chemical_melting_point_lt*** (*cif_core.dic 2.3*)

A temperature in kelvins below which the melting point (the temperature at which the crystalline solid changes to a liquid) lies. **_chemical.melting_point_gt** and **_chemical.melting_point_lt** allow a range of temperatures to be given. **_chemical.melting_point** should always be used in preference to these two items whenever possible.

The permitted range is $[0.0, \infty)$.

Related item: **_chemical.melting_point** (alternate). **[chemical]**

### _chemical.name_common (*text*)

***_chemical_name_common*** (*cif_core.dic 2.0.1*)

Trivial name by which the compound is commonly known.

Example: '1-bromoestradiol'. **[chemical]**

### _chemical.name_mineral (*text*)

***_chemical_name_mineral*** (*cif_core.dic 2.0.1*)

Mineral name accepted by the International Mineralogical Association. Use only for natural minerals. See also **_chemical.compound_source**.

Example: 'chalcopyrite'. **[chemical]**

### _chemical.name_structure_type (*text*)

***_chemical_name_structure_type*** (*cif_core.dic 2.0.1*)

Commonly used structure-type name. Usually only applied to minerals or inorganic compounds.

Examples: 'perovskite', 'sphalerite', 'A15'. **[chemical]**

### _chemical.name_systematic (*text*)

***_chemical_name_systematic*** (*cif_core.dic 2.0.1*)

IUPAC or *Chemical Abstracts* full name of the compound.

Example: '1-bromoestra-1,3,5(10)-triene-3,17\b-diol'. **[chemical]**

### _chemical.optical_rotation (*line*)

***_chemical_optical_rotation*** (*cif_core.dic 2.3*)

The optical rotation in solution of the compound is specified in the following format:

$$[\alpha]^{\mathrm{TEMP}}_{\mathrm{WAVE}} = \mathrm{SORT} \quad (c = \mathrm{CONC},\ \mathrm{SOLV}),$$

where TEMP is the temperature of the measurement in degrees Celsius, WAVE is an indication of the wavelength of the light used for the measurement, CONC is the concentration of the solution given as the mass of the substance in g per 100 ml of solution, SORT is the signed value (preceded by a + or a - sign) of $100\alpha/(lc)$, where $\alpha$ is the signed optical rotation in degrees measured in a cell of length $l$ in dm and $c$ is the value of CONC as defined above, and SOLV is the chemical formula of the solvent.

Example: '[\a]^25^~D~ = +108 (c = 3.42, CHCl~3~)'. **[chemical]**

### _chemical.properties_biological (*text*)

***_chemical_properties_biological*** (*cif_core.dic 2.3*)

A free-text description of the biological properties of the material.

Examples:

```
; diverse biological activities including use as a
  laxative and strong antibacterial activity against
  S. aureus and weak activity against
  cyclooxygenase-1 (COX-1)
;
; antibiotic activity against Bacillus subtilis
  (ATCC 6051) but no significant activity against
  Candida albicans (ATCC 14053), Aspergillus flavus
  (NRRL 6541) and Fusarium verticillioides (NRRL
  25457)
;
; weakly potent lipoxygenase nonredox inhibitor
;
; no influenza A virus sialidase inhibitory and
  plaque reduction activities
;
; low toxicity against Drosophila melanogaster
;
```

**[chemical]**

### _chemical.properties_physical (*text*)

***_chemical_properties_physical*** (*cif_core.dic 2.3*)

A free-text description of the physical properties of the material.

Examples: 'air-sensitive', 'moisture-sensitive', 'hygroscopic', 'deliquescent', 'oxygen-sensitive', 'photo-sensitive', 'pyrophoric', 'semiconductor', 'ferromagnetic at low temperature', 'paramagnetic and thermochromic'. **[chemical]**

### _chemical.temperature_decomposition (*float, su*)

***_chemical_temperature_decomposition*** (*cif_core.dic 2.3*)

The temperature in kelvins at which the solid decomposes.

The permitted range is $[0.0, \infty)$.

Related item: **_chemical.temperature_decomposition_esd** (associated esd) .

Example: '350'. **[chemical]**

### _chemical.temperature_decomposition_esd (*float*)

The estimated standard deviation of **_chemical.temperature_decomposition**.

Related item: **_chemical.temperature_decomposition** (associated value).

**[chemical]**

**_chemical.temperature_decomposition_gt** (*float*)
***_chemical_temperature_decomposition_gt*** (*cif_core.dic 2.3*)
A temperature in kelvins above which the solid is known to decompose. **_chemical.temperature_decomposition_gt** and **_chemical.temperature_decomposition_lt** allow a range of temperatures to be given. **_chemical.temperature_decomposition** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_chemical.temperature_decomposition** (alternate) .
Example: '350'. **[chemical]**

**_chemical.temperature_decomposition_lt** (*float*)
***_chemical_temperature_decomposition_lt*** (*cif_core.dic 2.3*)
A temperature in kelvins below which the solid is known to decompose. **_chemical.temperature_decomposition_gt** and **_chemical.temperature_decomposition_lt** allow a range of temperatures to be given. **_chemical.temperature_decomposition** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_chemical.temperature_decomposition** (alternate) .
Example: '350'. **[chemical]**

**_chemical.temperature_sublimation** (*float, su*)
***_chemical_temperature_sublimation*** (*cif_core.dic 2.3*)
The temperature in kelvins at which the solid sublimes.
The permitted range is $[0.0, \infty)$.
Related item: **_chemical.temperature_sublimation_esd** (associated esd) .
Example: '350'. **[chemical]**

**_chemical.temperature_sublimation_esd** (*float*)
The estimated standard deviation of **_chemical.temperature_sublimation**.
Related item: **_chemical.temperature_sublimation** (associated value).
**[chemical]**

**_chemical.temperature_sublimation_gt** (*float*)
***_chemical_temperature_sublimation_gt*** (*cif_core.dic 2.3*)
A temperature in kelvins above which the solid is known to sublime. **_chemical.temperature_sublimation_gt** and **_chemical.temperature_sublimation_lt** allow a range of temperatures to be given. **_chemical.temperature_sublimation** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_chemical.temperature_sublimation** (alternate) .
Example: '350'. **[chemical]**

**_chemical.temperature_sublimation_lt** (*float*)
***_chemical_temperature_sublimation_lt*** (*cif_core.dic 2.3*)
A temperature in kelvins below which the solid is known to sublime. **_chemical.temperature_sublimation_gt** and **_chemical.temperature_sublimation_lt** allow a range of temperatures to be given. **_chemical.temperature_sublimation** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_chemical.temperature_sublimation** (alternate) .
Example: '350'. **[chemical]**

## CHEMICAL_CONN_ATOM

Data items in the CHEMICAL_CONN_ATOM category would not, in general, be used in a macromolecular CIF. See instead the ENTITY data items. Data items in the CHEMICAL_CONN_ATOM and CHEMICAL_CONN_BOND categories record details about the two-dimensional (2D) chemical structure of the molecular species. They allow a 2D chemical diagram to be reconstructed for use in a publication or in a database search for structural and substructural relationships. The CHEMICAL_CONN_ATOM data items provide information about the chemical properties of the atoms in the structure. In cases where crystallographic and molecular symmetry elements coincide, they must also contain symmetry-generated atoms, so that the CHEMICAL_CONN_ATOM and CHEMICAL_CONN_BOND data items will always describe a complete chemical entity.
Category group(s): **inclusive_group**
**chemical_group**
Category key(s): **_chemical_conn_atom.number**

*Example 1 – based on data set DPTD of Yamin, Suwandi, Fun, Sivakumar & bin Shawkataly [Acta Cryst. (1996), C**52**, 951–953].*

```
loop_
_chemical_conn_atom.number
_chemical_conn_atom.type_symbol
_chemical_conn_atom.display_x
_chemical_conn_atom.display_y
_chemical_conn_atom.NCA
_chemical_conn_atom.NH
    1   S    .39  .81   1   0
    2   S    .39  .96   2   0
    3   N    .14  .88   3   0
    4   C    .33  .88   3   0
    5   C    .11  .96   2   2
    6   C    .03  .96   2   2
    7   C    .03  .80   2   2
    8   C    .11  .80   2   2
    9   S    .54  .81   1   0
    10  S    .54  .96   2   0
    11  N    .80  .88   3   0
    12  C    .60  .88   3   0
    13  C    .84  .96   2   2
    14  C    .91  .96   2   2
    15  C    .91  .80   2   2
    16  C    .84  .80   2   2
```

**_chemical_conn_atom.charge** (*int*)
***_chemical_conn_atom_charge*** (*cif_core.dic 2.0.1*)
The net integer charge assigned to this atom. This is the formal charge assignment normally found in chemical diagrams.
The permitted range is $[-8, 8]$. Where no value is given, the assumed value is '0'.
Examples: '1' (for an ammonium nitrogen), '-1' (for a chloride ion).
**[chemical_conn_atom]**

**_chemical_conn_atom.display_x** (*float*)
***_chemical_conn_atom_display_x*** (*cif_core.dic 2.0.1*)
The 2D Cartesian *x* coordinate of the position of this atom in a recognizable chemical diagram. The coordinate origin is at the lower left corner, the *x* axis is horizontal and the *y* axis is vertical. The coordinates must lie in the range 0.0 to 1.0. These coordinates can be obtained from projections of a suitable uncluttered view of the molecular structure.
The permitted range is [0.0, 1.0]. **[chemical_conn_atom]**

**_chemical_conn_atom.display_y** (*float*)
***_chemical_conn_atom_display_y*** (*cif_core.dic 2.0.1*)
The 2D Cartesian *y* coordinate of the position of this atom in a recognizable chemical diagram. The coordinate origin is at the lower left corner, the *x* axis is horizontal and the *y* axis is vertical. The coordinates must lie in the range 0.0 to 1.0. These coordinates can be obtained from projections of a suitable uncluttered view of the molecular structure.
The permitted range is [0.0, 1.0]. **[chemical_conn_atom]**

**_chemical_conn_atom.NCA** (*int*)
***_chemical_conn_atom_NCA*** (*cif_core.dic 2.0.1*)
The number of connected atoms excluding terminal hydrogen atoms.
The permitted range is $[0, \infty)$. **[chemical_conn_atom]**

**_chemical_conn_atom.NH** (*int*)
***_chemical_conn_atom_NH*** (*cif_core.dic 2.0.1*)
The total number of hydrogen atoms attached to this atom, regardless of whether they are included in the refinement or the ATOM_SITE list. This number is the same as **_atom_site.attached_hydrogens** only if none of the hydrogen atoms appear in the ATOM_SITE list.
The permitted range is $[0, \infty)$. **[chemical_conn_atom]**

***_chemical_conn_atom.number** (*int*)
***_chemical_conn_atom_number*** (*cif_core.dic 2.0.1*)
The chemical sequence number to be associated with this atom. Within an ATOM_SITE list, this number must match one of the **_atom_site.chemical_conn_number** values.
*The following item(s) have an equivalent role in their respective categories:*
***_atom_site.chemical_conn_number***,
***_chemical_conn_bond.atom_1***,
***_chemical_conn_bond.atom_2***.
The permitted range is $[1, \infty)$. **[chemical_conn_atom]**

***_chemical_conn_atom.type_symbol**
***_chemical_conn_atom_type_symbol*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_atom_type.symbol** in the ATOM_TYPE category.

## CHEMICAL_CONN_BOND

Data items in the CHEMICAL_CONN_BOND category would not, in general, be used in a macromolecular CIF. See instead the ENTITY data items. Data items in the CHEMICAL_CONN_ATOM and CHEMICAL_CONN_BOND categories record details about the two-dimensional (2D) chemical structure of the molecular species. They allow a 2D chemical diagram to be reconstructed for use in a publication or in a database search for structural and substructural relationships. The CHEMICAL_CONN_BOND data items specify the connections between the atoms in the CHEMICAL_CONN_ATOM list and the nature of the chemical bond between these atoms.
Category group(s): **inclusive_group**
**chemical_group**
Category key(s): **_chemical_conn_bond.atom_1**
**_chemical_conn_bond.atom_2**

*Example 1 – based on data set DPTD of Yamin, Suwandi, Fun, Sivakumar & bin Shawkataly [Acta Cryst. (1996), C**52**, 951–953].*

```
loop_
_chemical_conn_bond.atom_1
_chemical_conn_bond.atom_2
_chemical_conn_bond.type
   4     1     doub      4     3     sing
   4     2     sing      5     3     sing
   6     5     sing      7     6     sing
   8     7     sing      8     3     sing
   10    2     sing      12    9     doub
   12    11    sing      12    10    sing
   13    11    sing      14    13    sing
   15    14    sing      16    15    sing
   16    11    sing      17    5     sing
   18    5     sing      19    6     sing
   20    6     sing      21    7     sing
   22    7     sing      23    8     sing
   24    8     sing      25    13    sing
   26    13    sing      27    14    sing
   28    14    sing      29    15    sing
   30    15    sing      31    16    sing
   32    16    sing
```

***_chemical_conn_bond.atom_1**
***_chemical_conn_bond_atom_1*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_chemical_conn_atom.number** in the CHEMICAL_CONN_ATOM category.

***_chemical_conn_bond.atom_2**
***_chemical_conn_bond_atom_2*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_chemical_conn_atom.number** in the CHEMICAL_CONN_ATOM category.

**_chemical_conn_bond.type** (*ucode*)
***_chemical_conn_bond_type*** (*cif_core.dic 2.0.1*)
The chemical bond type associated with the connection between the two sites **_chemical_conn_bond.atom_1** and **_chemical_conn_bond.atom_2**.
The data value must be one of the following:

| | |
|---|---|
| `sing` | single bond |
| `doub` | double bond |
| `trip` | triple bond |
| `quad` | quadruple bond |
| `arom` | aromatic bond |
| `poly` | polymeric bond |
| `delo` | delocalized double bond |
| `pi` | $\pi$ bond |

Where no value is given, the assumed value is '`sing`'. **[chemical_conn_bond]**

## CHEMICAL_FORMULA

Data items in the CHEMICAL_FORMULA category would not, in general, be used in a macromolecular CIF. See instead the ENTITY data items. Data items in the CHEMICAL_FORMULA category specify the composition and chemical properties of the compound. The formula data items must agree with those that specify the density, unit-cell and $Z$ values. The following rules apply to the construction of the data items **_chemical_formula.analytical**, **_chemical_formula.structural** and **_chemical_formula.sum**. For the data item **_chemical_formula.moiety**, the formula construction is broken up into residues or moieties, *i.e.* groups of atoms that form a molecular unit or molecular ion. The rules given below apply within each moiety but different requirements apply to the way that moieties are connected (see **_chemical_formula.moiety**). (1) Only recognized element symbols may be used. (2) Each element symbol is followed by a 'count' number. A count of '1' may be omitted. (3) A space or parenthesis must separate each cluster of (element symbol + count). (4) Where a group of elements is enclosed in parentheses, the multiplier for the group must follow the closing parenthesis. That is, all element and group multipliers are assumed to be printed as subscripted numbers. (An exception to this rule exists for **_chemical_formula.moiety** formulae where pre- and post-multipliers are permitted for molecular units.) (5) Unless the elements are ordered in a manner that corresponds to their chemical structure, as in **_chemical_formula.structural**, the order of the elements within any group or moiety should be: C, then H, then the other elements in alphabetical order of their symbol. This is the 'Hill' system used by *Chemical Abstracts*. This ordering is used in **_chemical_formula.moiety** and **_chemical_formula.sum**.
Category group(s): **inclusive_group**
**chemical_group**
Category key(s): **_chemical_formula.entry_id**

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [(1991). Acta Cryst. C**47**, 2276–2277].*

```
_chemical_formula.entry_id          'TOZ'
_chemical_formula.moiety            'C18 H25 N O3'
_chemical_formula.sum               'C18 H25 N O3'
_chemical_formula.weight            303.40
```

### _chemical_formula.analytical (*text*)

***_chemical_formula_analytical*** (*cif_core.dic 2.0.1*)

Formula determined by standard chemical analysis including trace elements. See the CHEMICAL_FORMULA category description for rules for writing chemical formulae. Parentheses are used only for standard uncertainties (estimated standard deviations).

Example: 'Fe2.45(2) Ni1.60(3) S4'. **[chemical_formula]**

### *_chemical_formula.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### _chemical_formula.iupac (*text*)

***_chemical_formula_iupac*** (*cif_core.dic 2.0.1*)

Formula expressed in conformance with IUPAC rules for inorganic and metal-organic compounds where these conflict with the rules for any other CHEMICAL_FORMULA entries. Typically used for formatting a formula in accordance with journal rules. This should appear in the data block in addition to the most appropriate of the other CHEMICAL_FORMULA data names.

Reference: IUPAC (1990). *Nomenclature of Inorganic Chemistry*. Oxford: Blackwell Scientific Publications.

Example: '[Co Re (C12 H22 P)2 (C O)6].0.5C H3 O H'. **[chemical_formula]**

### _chemical_formula.moiety (*text*)

***_chemical_formula_moiety*** (*cif_core.dic 2.0.1*)

Formula with each discrete bonded residue or ion shown as a separate moiety. See the CHEMICAL_FORMULA category description for rules for writing chemical formulae. In addition to the general formulae requirements, the following rules apply: (1) Moieties are separated by commas ','. (2) The order of elements within a moiety follows general rule (5) in the CHEMICAL_FORMULA category description. (3) Parentheses are not used within moieties but may surround a moiety. Parentheses may not be nested. (4) Charges should be placed at the end of the moiety. The charge '+' or '-' may be preceded by a numerical multiplier and should be separated from the last (element symbol + count) by a space. Pre- or post-multipliers may be used for individual moieties.

Examples: 'C7 H4 Cl Hg N O3 S', 'C12 H17 N4 O S 1+, C6 H2 N3 O7 1-', 'C12 H16 N2 O6, 5(H2 O1)', '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'. **[chemical_formula]**

### _chemical_formula.structural (*text*)

***_chemical_formula_structural*** (*cif_core.dic 2.0.1*)

See the CHEMICAL_FORMULA category description for the rules for writing chemical formulae for inorganics, organometallics, metal complexes *etc.*, in which bonded groups are preserved as discrete entities within parentheses, with post-multipliers as required. The order of the elements should give as much information as possible about the chemical structure. Parentheses may be used and nested as required. This formula should correspond to the structure as actually reported, *i.e.* trace elements not included in atom-type and atom-site data should not be included in this formula (see also **_chemical_formula.analytical**).

Examples: 'Ca ((Cl O3)2 O)2 (H2 O)6', '(Pt (N H3)2 (C5 H7 N3 O)2) (Cl O4)2'. **[chemical_formula]**

### _chemical_formula.sum (*text*)

***_chemical_formula_sum*** (*cif_core.dic 2.0.1*)

See the CHEMICAL_FORMULA category description for the rules for writing chemical formulae in which all discrete bonded residues and ions are summed over the constituent elements, following the ordering given in general rule (5) in the CHEMICAL_FORMULA category description. Parentheses are not normally used.

Example: 'C18 H19 N7 O8 S'. **[chemical_formula]**

### _chemical_formula.weight (*float*)

***_chemical_formula_weight*** (*cif_core.dic 2.0.1*)

Formula mass in daltons. This mass should correspond to the formulae given under **_chemical_formula.structural**, **_chemical_formula.moiety** or **_chemical_formula.sum** and, together with the $Z$ value and cell parameters, should yield the density given as **_exptl_crystal.density_diffrn**.

The permitted range is $[1.0, \infty)$. **[chemical_formula]**

### _chemical_formula.weight_meas (*float*)

***_chemical_formula_weight_meas*** (*cif_core.dic 2.0.1*)

Formula mass in daltons measured by a non-diffraction experiment.

The permitted range is $[1.0, \infty)$. **[chemical_formula]**

## CITATION

Data items in the CITATION category record details about the literature cited as being relevant to the contents of the data block.

Category group(s): **inclusive_group**
**citation_group**

Category key(s): **_citation.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_citation.id
_citation.coordinate_linkage
_citation.title
_citation.country
_citation.journal_abbrev
_citation.journal_volume
_citation.journal_issue
_citation.page_first
_citation.page_last
_citation.year
_citation.journal_id_ASTM
_citation.journal_id_ISSN
_citation.journal_id_CSD
_citation.book_title
_citation.book_publisher
_citation.book_id_ISBN
_citation.details
  primary  yes
; Crystallographic analysis of a complex between human
  immunodeficiency virus type 1 protease and acetyl-pepstatin
  at 2.0-Angstroms resolution.
;
  US  'J. Biol. Chem.'  265  .  14209  14219  1990
  HBCHA3  0021-9258  071  .  .  .
; The publication that directly relates to this coordinate
  set.
;
  2  no
; Three-dimensional structure of aspartyl-protease from human
  immunodeficiency virus HIV-1.
;
  UK  'Nature'  337  .  615  619  1989
  NATUAS  0028-0836  006  .  .  .
; Determination of the structure of the unliganded enzyme.
;
  3 no
; Crystallization of the aspartylprotease from human
  immunodeficiency virus, HIV-1.
;
  US  'J. Biol. Chem.'  264  .  1919  1921  1989
  HBCHA3  0021-9258  071  .  .  .
; Crystallization of the unliganded enzyme.
;
  4 no
; Human immunodeficiency virus protease. Bacterial expression
  and characterization of the purified aspartic protease.
;
  US  'J. Biol. Chem.'  264  .  2307  2312  1989
  HBCHA3  0021-9258  071  .  .  .
; Expression and purification of the enzyme.
;
```

**_citation.abstract** (*text*)
***_citation_abstract*** (*cif_core.dic 2.0.1*)
Abstract for the citation. This is used most when the citation is extracted from a bibliographic database that contains full text or abstract information.
**[citation]**

**_citation.abstract_id_CAS** (*text*)
***_citation_abstract_id_CAS*** (*cif_core.dic 2.0.1*)
The *Chemical Abstracts* Service (CAS) abstract identifier; relevant for journal articles.
**[citation]**

**_citation.book_id_ISBN** (*line*)
***_citation_book_id_ISBN*** (*cif_core.dic 2.0.1*)
The International Standard Book Number (ISBN) code assigned to the book cited; relevant for books or book chapters.
**[citation]**

**_citation.book_publisher** (*text*)
***_citation_book_publisher*** (*cif_core.dic 2.0.1*)
The name of the publisher of the citation; relevant for books or book chapters.
Example: 'John Wiley and Sons'. **[citation]**

**_citation.book_publisher_city** (*text*)
***_citation_book_publisher_city*** (*cif_core.dic 2.0.1*)
The location of the publisher of the citation; relevant for books or book chapters.
Example: 'London'. **[citation]**

**_citation.book_title** (*text*)
***_citation_book_title*** (*cif_core.dic 2.0.1*)
The title of the book in which the citation appeared; relevant for books or book chapters.
**[citation]**

**_citation.coordinate_linkage** (*ucode*)
***_citation_coordinate_linkage*** (*cif_core.dic 2.0.1*)
**_citation.coordinate_linkage** states whether this citation is concerned with precisely the set of coordinates given in the data block. If, for instance, the publication described the same structure, but the coordinates had undergone further refinement prior to the creation of the data block, the value of this data item would be 'no'.
The data value must be one of the following:

| | |
|---|---|
| no | citation unrelated to current coordinates |
| n | abbreviation for 'no' |
| yes | citation related to current coordinates |
| y | abbreviation for 'yes' |

**[citation]**

**_citation.country** (*line*)
***_citation_country*** (*cif_core.dic 2.0.1*)
The country of publication; relevant for books and book chapters.
**[citation]**

**_citation.database_id_CSD** (*code*)
***_citation_database_id_CSD*** (*cif_core.dic 2.3*)
Identifier ('refcode') of the database record in the Cambridge Structural Database that contains details of the cited structure.
Example: 'LEKKUH'. **[citation]**

**_citation.database_id_Medline** (*int*)
***_citation_database_id_Medline*** (*cif_core.dic 2.0.1*)
Accession number used by Medline to categorize a specific bibliographic entry.
The permitted range is $[1, \infty)$.
Example: '89064067'. **[citation]**

**_citation.details** (*text*)
***_citation_special_details*** (*cif_core.dic 2.0.1*)
A description of special aspects of the relationship of the contents of the data block to the literature item cited.
Examples:

```
; citation relates to this precise
  coordinate set
;
; citation relates to earlier low-resolution
  structure
;
; citation relates to further refinement of
  structure reported in citation 2
;
```

**[citation]**

***_citation.id** (*code*)
***_citation_id*** (*cif_core.dic 2.0.1*)
The value of **_citation.id** must uniquely identify a record in the CITATION list. The **_citation.id** 'primary' should be used to indicate the citation that the author(s) consider to be the most pertinent to the contents of the data block. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_citation_author.citation_id***,
***_citation_editor.citation_id***,
***_software.citation_id***.
Examples: 'primary', '1', '2'. **[citation]**

**_citation.journal_abbrev** (*line*)
***_citation_journal_abbrev*** (*cif_core.dic 2.0.1*)
Abbreviated name of the cited journal as given in the *Chemical Abstracts* Service *Source Index*.
Example: 'J. Mol. Biol.'. **[citation]**

**_citation.journal_full** (*text*)
***_citation_journal_full*** (*cif_core.dic 2.0.1*)
Full name of the cited journal; relevant for journal articles.
Example: 'Journal of Molecular Biology'. **[citation]**

**_citation.journal_id_ASTM** (*line*)
***_citation_journal_id_ASTM*** (*cif_core.dic 2.0.1*)
The American Society for Testing and Materials (ASTM) code assigned to the journal cited (also referred to as the CODEN designator of the *Chemical Abstracts* Service); relevant for journal articles.
**[citation]**

**_citation.journal_id_CSD** (*line*)
***_citation_journal_id_CSD*** (*cif_core.dic 2.0.1*)
The Cambridge Structural Database (CSD) code assigned to the journal cited; relevant for journal articles. This is also the system used at the Protein Data Bank (PDB).
Example: '0070'. **[citation]**

**_citation.journal_id_ISSN** (*line*)
***_citation_journal_id_ISSN*** (*cif_core.dic 2.0.1*)
The International Standard Serial Number (ISSN) code assigned to the journal cited; relevant for journal articles.
**[citation]**

**_citation.journal_issue** (*line*)
***_citation_journal_issue*** (*cif_core.dic 2.0.1*)
Issue number of the journal cited; relevant for journal articles.
Example: '2'. **[citation]**

**_citation.journal_volume** (*line*)
***_citation_journal_volume*** (*cif_core.dic 2.0.1*)
Volume number of the journal cited; relevant for journal articles.
Example: '174'. **[citation]**

**_citation.language** (*line*)
***_citation_language*** (*cif_core.dic 2.0.1*)
Language in which the cited article is written.
Example: 'German'. **[citation]**

**_citation.page_first** (*line*)
***_citation_page_first*** (*cif_core.dic 2.0.1*)
The first page of the citation; relevant for journal articles, books and book chapters.
**[citation]**

**_citation.page_last** (*line*)
***_citation_page_last*** (*cif_core.dic 2.0.1*)
The last page of the citation; relevant for journal articles, books and book chapters.
**[citation]**

**_citation.title** (*text*)
***_citation_title*** (*cif_core.dic 2.0.1*)
The title of the citation; relevant for journal articles, books and book chapters.
Example:
```
; Structure of diferric duck ovotransferrin at 2.35 \%A
resolution.
;
```
**[citation]**

**_citation.year** (*int*)
***_citation_year*** (*cif_core.dic 2.0.1*)
The year of the citation; relevant for journal articles, books and book chapters.
Example: '1984'. **[citation]**

## CITATION_AUTHOR

Data items in the CITATION_AUTHOR category record details about the authors associated with the citations in the CITATION list.
Category group(s): **inclusive_group**
**citation_group**
Category key(s): **_citation_author.citation_id**
**_citation_author.name**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_citation_author.citation_id
_citation_author.ordinal
_citation_author.name
  primary  1  'Fitzgerald, P.M.D.'
  primary  2  'McKeever, B.M.'
  primary  3  'Van Middlesworth, J.F.'
  primary  4  'Springer, J.P.'
  primary  5  'Heimbach, J.C.'
  primary  6  'Leu, C.-T.'
  primary  7  'Herber, W.K.'
  primary  8  'Dixon, R.A.F.'
  primary  9  'Darke, P.L.'
  2        1  'Navia, M.A.'
  2        2  'Fitzgerald, P.M.D.'
  2        3  'McKeever, B.M.'
  2        4  'Leu, C.-T.'
  2        5  'Heimbach, J.C.'
  2        6  'Herber, W.K.'
  2        7  'Sigal, I.S.'
  2        8  'Darke, P.L.'
  2        9  'Springer, J.P.'
  3        1  'McKeever, B.M.'
  3        2  'Navia, M.A.'
  3        3  'Fitzgerald, P.M.D.'
  3        4  'Springer, J.P.'
  3        5  'Leu, C.-T.'
  3        6  'Heimbach, J.C.'
  3        7  'Herber, W.K.'
  3        8  'Sigal, I.S.'
  3        9  'Darke, P.L.'
  4        1  'Darke, P.L.'
  4        2  'Leu, C.-T.'
  4        3  'Davis, L.J.'
  4        4  'Heimbach, J.C.'
  4        5  'Diehl, R.E.'
  4        6  'Hill, W.S.'
  4        7  'Dixon, R.A.F.'
  4        8  'Sigal, I.S.'
```

*__citation_author.citation_id**
***_citation_author_citation_id*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_citation.id** in the CITATION category.

*__citation_author.name** (*line*)
***_citation_author_name*** (*cif_core.dic 2.0.1*)
Name of an author of the citation; relevant for journal articles, books and book chapters. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).
Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[citation_author]**

**_citation_author.ordinal** (*int*)
***_citation_author_ordinal*** (*cif_core.dic 2.0.1*)
This data item defines the order of the author's name in the list of authors of a citation.
**[citation_author]**

## CITATION_EDITOR

Data items in the CITATION_EDITOR category record details about the editors associated with the books or book chapters cited in the CITATION list.

Category group(s): **inclusive_group**
**citation_group**
Category key(s): **_citation_editor.citation_id**
**_citation_editor.name**

*Example 1 – hypothetical example.*

```
loop_
_citation_editor.citation_id
_citation_editor.name
  5        'McKeever, B.M.'
  5        'Navia, M.A.'
  5        'Fitzgerald, P.M.D.'
  5        'Springer, J.P.'
```

* **_citation_editor.citation_id**
***_citation_editor_citation_id*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_citation.id** in the CITATION category.

**_citation_editor.name** (*line*)
***_citation_editor_name*** (*cif_core.dic 2.0.1*)
Names of an editor of the citation; relevant for books and book chapters. The family name(s), followed by a comma and including any dynastic components, precedes the first name(s) or initial(s).
Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[citation_editor]**

**_citation_editor.ordinal** (*int*)
***_citation_editor_ordinal*** (*cif_core.dic 2.0.1*)
This data item defines the order of the editor's name in the list of editors of a citation.
**[citation_editor]**

## COMPUTING

Data items in the COMPUTING category record details about the computer programs used in the crystal structure analysis. Data items in this category would not, in general, be used in a macromolecular CIF. The category SOFTWARE, which allows a more detailed description of computer programs and their attributes to be given, would be used instead.

Category group(s): **inclusive_group**
**computing_group**
Category key(s): **_computing.entry_id**

*Example 1 – Rodrìguez-Romera, Ruiz-Pérez & Solans [Acta Cryst. (1996), C52, 1415–1417].*

```
_computing.data_collection      'CAD-4 (Enraf-Nonius, 1989)'
_computing.cell_refinement      'CAD-4 (Enraf-Nonius, 1989)'
_computing.data_reduction       'CFEO (Solans, 1978)'
_computing.structure_solution   'SHELXS86 (Sheldrick, 1990)'
_computing.structure_refinement 'SHELXL93 (Sheldrick, 1993)'
_computing.molecular_graphics   'ORTEPII (Johnson, 1976)'
_computing.publication_material 'PARST (Nardelli, 1983)'
```

**_computing.cell_refinement** (*text*)
***_computing_cell_refinement*** (*cif_core.dic 2.0.1*)
Software used for cell refinement. Give the program or package name and a brief reference.
Example: 'CAD4 (Enraf-Nonius, 1989)'. **[computing]**

**_computing.data_collection** (*text*)
***_computing_data_collection*** (*cif_core.dic 2.0.1*)
Software used for data collection. Give the program or package name and a brief reference.
Example: 'CAD4 (Enraf-Nonius, 1989)'. **[computing]**

**_computing.data_reduction** (*text*)
***_computing_data_reduction*** (*cif_core.dic 2.0.1*)
Software used for data reduction. Give the program or package name and a brief reference.
Example: 'DIFDAT, SORTRF, ADDREF (Hall & Stewart, 1990)'.
**[computing]**

* **_computing.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_computing.molecular_graphics** (*text*)
***_computing_molecular_graphics*** (*cif_core.dic 2.0.1*)
Software used for molecular graphics. Give the program or package name and a brief reference.
Example: 'FRODO (Jones, 1986), ORTEP (Johnson, 1965)'. **[computing]**

**_computing.publication_material** (*text*)
***_computing_publication_material*** (*cif_core.dic 2.0.1*)
Software used for generating material for publication. Give the program or package name and a brief reference.
**[computing]**

**_computing.structure_refinement** (*text*)
***_computing_structure_refinement*** (*cif_core.dic 2.0.1*)
Software used for refinement of the structure. Give the program or package name and a brief reference.
Examples: 'SHELX85 (Sheldrick, 1985)', 'X-PLOR (Brunger, 1992)'.
**[computing]**

**_computing.structure_solution** (*text*)
***_computing_structure_solution*** (*cif_core.dic 2.0.1*)
Software used for solution of the structure. Give the program or package name and a brief reference.
Example: 'SHELX85 (Sheldrick, 1985)'. **[computing]**

## DATABASE

Data items in the DATABASE category have been superseded by data items in the DATABASE_2 category. They are included here only for compliance with older CIFs.

Category group(s): **inclusive_group**
**compliance_group**
Category key(s): **_database.entry_id**

**_database.code_CAS** (*line*)
***_database_code_CAS*** (*cif_core.dic 2.3*)
The code assigned by *Chemical Abstracts*.
**[database]**

**_database.code_CSD** (*line*)
***_database_code_CSD*** (*cif_core.dic 2.3*)
The code assigned by the Cambridge Structural Database.
**[database]**

**_database.code_ICSD** (*line*)
***_database_code_ICSD*** (*cif_core.dic 2.3*)
The code assigned by the Inorganic Crystal Structure Database.
**[database]**

**_database.code_MDF** (*line*)
***_database_code_MDF*** (*cif_core.dic 2.3*)
The code assigned by the Metals Data File.
**[database]**

**_database.code_NBS** (*line*)
***_database_code_NBS*** (*cif_core.dic 2.3*)
The code assigned by the NBS (NIST) Crystal Data Database.
**[database]**

**_database.code_PDB** (*line*)
***_database_code_PDB*** (*cif_core.dic 2.3*)
The code assigned by the Protein Data Bank.
**[database]**

**_database.code_PDF** (*line*)
***_database_code_PDF*** (*cif_core.dic 2.3*)
The code assigned by the Powder Diffraction File (JCPDS/ICDD).
**[database]**

**_database.code_depnum_ccdc_archive** (*line*)
***_database_code_depnum_ccdc_archive*** (*cif_core.dic 2.3*)
Deposition numbers assigned by the Cambridge Crystallographic Data Centre (CCDC) to files containing structural information archived by the CCDC.
**[database]**

**_database.code_depnum_ccdc_fiz** (*line*)
***_database_code_depnum_ccdc_fiz*** (*cif_core.dic 2.3*)
Deposition numbers assigned by the Fachinformationszentrum Karlsruhe (FIZ) to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).
**[database]**

**_database.code_depnum_ccdc_journal** (*line*)
***_database_code_depnum_ccdc_journal*** (*cif_core.dic 2.3*)
Deposition numbers assigned by various journals to files containing structural information archived by the Cambridge Crystallographic Data Centre (CCDC).
**[database]**

**_database.CSD_history** (*text*)
***_database_CSD_history*** (*cif_core.dic 2.3*)
A history of changes made by the Cambridge Crystallographic Data Centre and incorporated into the Cambridge Structural Database (CSD).
**[database]**

***_database.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_database.journal_ASTM** (*line*)
***_database_journal_ASTM*** (*cif_core.dic 2.0.1*)
The ASTM CODEN designator for a journal as given in the *Chemical Source List* maintained by the *Chemical Abstracts* Service.
**[database]**

**_database.journal_CSD** (*line*)
***_database_journal_CSD*** (*cif_core.dic 2.0.1*)
The journal code used in the Cambridge Structural Database.
**[database]**

## DATABASE_2

Data items in the DATABASE_2 category record details about the database identifiers of the data block. These data items are assigned by database managers and should only appear in a data block if they originate from that source. The name of this category, DATABASE_2, arose because the category name DATABASE was already in use in the core CIF dictionary, but was used differently from the way it needed to be used in the mmCIF dictionary. Since CIF data names cannot be changed once they have been adopted, a new category had to be created.

Category group(s): **inclusive_group**
**database_group**
Category key(s): **_database_2.database_id**
**_database_2.database_code**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_database_2.database_id       'PDB'
_database_2.database_code     '5HVP'
```

***_database_2.database_code** (*line*)
The code assigned by the database identified in **_database_2.database_id**.
Related items: **_database.code_CAS** (replaces),
**_database.code_CSD** (replaces),
**_database.code_ICSD** (replaces),
**_database.code_MDF** (replaces),
**_database.code_NBS** (replaces),
**_database.code_PDF** (replaces) .
Examples: '1ABC', 'ABCDEF'. **[database_2]**

***_database_2.database_id** (*ucode*)
An abbreviation that identifies the database.
Related items: **_database.code_CAS** (replaces),
**_database.code_CSD** (replaces),
**_database.code_ICSD** (replaces),
**_database.code_MDF** (replaces),
**_database.code_NBS** (replaces),
**_database.code_PDF** (replaces).
The data value must be one of the following:

| | |
|---|---|
| CAS | *Chemical Abstracts* |
| CSD | Cambridge Structural Database (organic and metal-organic compounds) |
| ICSD | Inorganic Crystal Structure Database |
| MDF | Metals Data File (metal structures) |
| NDB | Nucleic Acid Database |
| NBS | NBS (NIST) Crystal Data Database (lattice parameters) |
| PDB | Protein Data Bank |
| PDF | Powder Diffraction File (JCPDS/ICDD) |
| RCSB | Research Collaboratory for Structural Bioinformatics |
| EBI | European Bioinformatics Institute |

**[database_2]**

## DATABASE_PDB_CAVEAT

Data items in the DATABASE_PDB_CAVEAT category record details about features of the data block flagged as 'caveats' by the Protein Data Bank (PDB). These data items are included only for consistency with PDB format files. They should appear in a data block only if that data block was created by reformatting a PDB format file.

Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_caveat.id**

*Example 1 – hypothetical example.*

```
loop_
_database_PDB_caveat.id
_database_PDB_caveat.text
1
; THE CRYSTAL TRANSFORMATION IS IN ERROR BUT IS
;
2
; UNCORRECTABLE AT THIS TIME
;
```

***_database_PDB_caveat.id** (*int*)
A unique identifier for the PDB caveat record.

**[database_PDB_caveat]**

**_database_PDB_caveat.text** (*text*)
The full text of the PDB caveat record.

**[database_PDB_caveat]**

## DATABASE_PDB_MATRIX

The DATABASE_PDB_MATRIX category provides placeholders for transformation matrices and vectors used by the Protein Data Bank (PDB). These data items are included only for consistency with older PDB format files. They should appear in a data block only if that data block was created by reformatting a PDB format file.

Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_matrix.entry_id**

***_database_PDB_matrix.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_database_PDB_matrix.origx[1][1]** (*float*)
The [1][1] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[1][2]** (*float*)
The [1][2] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[1][3]** (*float*)
The [1][3] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[2][1]** (*float*)
The [2][1] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[2][2]** (*float*)
The [2][2] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[2][3]** (*float*)
The [2][3] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[3][1]** (*float*)
The [3][1] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[3][2]** (*float*)
The [3][2] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx[3][3]** (*float*)
The [3][3] element of the PDB ORIGX matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx_vector[1]** (*float*)
The [1] element of the PDB ORIGX vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx_vector[2]** (*float*)
The [2] element of the PDB ORIGX vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.origx_vector[3]** (*float*)
The [3] element of the PDB ORIGX vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[1][1]** (*float*)
The [1][1] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[1][2]** (*float*)
The [1][2] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[1][3]** (*float*)
The [1][3] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[2][1]** (*float*)
The [2][1] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[2][2]** (*float*)
The [2][2] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[2][3]** (*float*)
The [2][3] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[3][1]** (*float*)
The [3][1] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[3][2]** (*float*)
The [3][2] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale[3][3]** (*float*)
The [3][3] element of the PDB SCALE matrix.
Where no value is given, the assumed value is '1.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale_vector[1]** (*float*)
The [1] element of the PDB SCALE vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale_vector[2]** (*float*)
The [2] element of the PDB SCALE vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

**_database_PDB_matrix.scale_vector[3]** (*float*)
The [3] element of the PDB SCALE vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_matrix]**

## DATABASE_PDB_REMARK

Data items in the DATABASE_PDB_REMARK category record details about the data block as archived by the Protein Data Bank (PDB). Some data appearing in PDB REMARK records can be algorithmically extracted into the appropriate data items in the data block. These data items are included only for consistency with older PDB format files. They should appear in a data block only if that data block was created by reformatting a PDB format file.
Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_remark.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_database_PDB_remark.id
_database_PDB_remark.text
3
; REFINEMENT. BY THE RESTRAINED LEAST-SQUARES PROCEDURE OF J.
  KONNERT AND W. HENDRICKSON (PROGRAM *PROLSQ*).  THE R
  VALUE IS 0.176 FOR 12901 REFLECTIONS IN THE RESOLUTION
  RANGE 8.0 TO 2.0 ANGSTROMS WITH I .GT. SIGMA(I).

  RMS DEVIATIONS FROM IDEAL VALUES (THE VALUES OF
  SIGMA, IN PARENTHESES, ARE THE INPUT ESTIMATED
  STANDARD DEVIATIONS THAT DETERMINE THE RELATIVE
  WEIGHTS OF THE CORRESPONDING RESTRAINTS)
  DISTANCE RESTRAINTS (ANGSTROMS)
  BOND DISTANCE                          0.018(0.020)
  ANGLE DISTANCE                         0.038(0.030)
  PLANAR 1-4 DISTANCE                    0.043(0.040)
  PLANE RESTRAINT (ANGSTROMS)              0.015(0.020)
  CHIRAL-CENTER RESTRAINT (ANGSTROMS**3)     0.177(0.150)
  NON-BONDED CONTACT RESTRAINTS (ANGSTROMS)
  SINGLE TORSION CONTACT                 0.216(0.500)
  MULTIPLE TORSION CONTACT               0.207(0.500)
  POSSIBLE HYDROGEN BOND                 0.245(0.500)
  CONFORMATIONAL TORSION ANGLE RESTRAINT (DEGREES)
  PLANAR (OMEGA)                           2.6(3.0)
  STAGGERED                               17.4(15.0)
  ORTHONORMAL                             18.1(20.0)
;
4
; THE TWO CHAINS OF THE DIMERIC ENZYME HAS BEEN ASSIGNED THE
  THE CHAIN INDICATORS *A* AND *B*.
;
#  - - - - data truncated for brevity - - - -
```

***_database_PDB_remark.id** (*int*)
A unique identifier for the PDB remark record.
**[database_PDB_remark]**

**_database_PDB_remark.text** (*text*)
The full text of the PDB remark record.
**[database_PDB_remark]**

## DATABASE_PDB_REV

Data items in the DATABASE_PDB_REV category record details about the history of the data block as archived by the Protein Data Bank (PDB). These data items are assigned by the PDB database managers and should only appear in a data block if they originate from that source.
Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_rev.num**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_database_PDB_rev.num
_database_PDB_rev.author_name
_database_PDB_rev.date
_database_PDB_rev.date_original
_database_PDB_rev.status
_database_PDB_rev.mod_type
  1  'Fitzgerald, Paula M.D' 1991-10-15  1990-04-30
  'full release'  0
```

**_database_PDB_rev.author_name** (*line*)
The name of the person responsible for submitting this revision to the PDB. The family name(s) followed by a comma precedes the first name(s) or initial(s).
Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[database_PDB_rev]**

**_database_PDB_rev.date** (*yyyy-mm-dd*)
Date the PDB revision took place. Taken from the REVDAT record.
**[database_PDB_rev]**

**_database_PDB_rev.date_original** (*yyyy-mm-dd*)
Date the entry first entered the PDB database in the form *yyyy-mm-dd*. Taken from the PDB HEADER record.
Example: '1980-08-21'. **[database_PDB_rev]**

**_database_PDB_rev.mod_type** (*int*)
Taken from the REVDAT record. Refer to the Protein Data Bank format description at http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html for details.
The data value must be one of the following:

| | |
|---|---|
| 0 | initial entry |
| 1 | all other types of modification |
| 2 | modifications to CONECT records |
| 3 | modifications affecting the coordinates or their transforms (CRYST1, ORIGX, SCALE, MTRIX, TVECT, ATOM, HETATM, SIGATM records) |
| 4 | layer 1 to layer 2 revision which may affect all record types |
| 5 | data uniformity processing |

**[database_PDB_rev]**

***_database_PDB_rev.num** (*int*)
The value of **_database_PDB_rev.num** must uniquely and sequentially identify a record in the DATABASE_PDB_REV list. Note that this item must be a number and that modification numbers are assigned in increasing numerical order.
*The following item(s) have an equivalent role in their respective categories:*
***_database_PDB_rev_record.rev_num***. **[database_PDB_rev]**

**_database_PDB_rev.replaced_by** (*line*)
The PDB code for a subsequent PDB entry that replaced the PDB file corresponding to this data block.
**[database_PDB_rev]**

**_database_PDB_rev.replaces** (*line*)
The PDB code for a previous PDB entry that was replaced by the PDB file corresponding to this data block.
**[database_PDB_rev]**

**_database_PDB_rev.status** (*uline*)
The status of this revision.
The data value must be one of the following:
'in preparation'
prerelease
'full release'
obsolete
**[database_PDB_rev]**

## DATABASE_PDB_REV_RECORD

Data items in the DATABASE_PDB_REV_RECORD category record details about specific record types that were changed in a given revision of a PDB entry. These data items are assigned by the PDB database managers and should only appear in a data block if they originate from that source.
Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_rev_record.rev_num**
**_database_PDB_rev_record.type**

*Example 1 – hypothetical example.*

```
loop_
_database_PDB_rev_record.rev_num
_database_PDB_rev_record.type
_database_PDB_rev_record.details
  1  CONECT
; Error fix - incorrect connection between
  atoms 2312 and 2317
;
  2  MATRIX  'For consistency with 1995-08-04 style-guide'
  3  ORIGX   'Based on new data from author'
```

**_database_PDB_rev_record.details** (*text*)
A description of special aspects of the revision of records in this PDB entry.
Examples: 'Based on new data from author',
'For consistency with 1995-08-04 style-guide',
'For consistency with structural class'.
**[database_PDB_rev_record]**

***_database_PDB_rev_record.rev_num**
This data item is a pointer to **_database_PDB_rev.num** in the DATABASE_PDB_REV category.

***_database_PDB_rev_record.type** (*line*)
The types of records that were changed in this revision to a PDB entry.
Examples: 'CRYST1', 'SCALE', 'MTRIX', 'ATOM', 'HETATM'.
**[database_PDB_rev_record]**

## DATABASE_PDB_TVECT

The DATABASE_PDB_TVECT category provides placeholders for the TVECT matrices and vectors used by the Protein Data Bank (PDB). These data items are included only for consistency with older PDB format files. They should appear in a data block only if the data block was created by reformatting a PDB format file.
Category group(s): **inclusive_group**
**database_group**
**pdb_group**
Category key(s): **_database_PDB_tvect.id**

**_database_PDB_tvect.details** (*text*)
A description of special aspects of this TVECT.
**[database_PDB_tvect]**

***_database_PDB_tvect.id** (*code*)
The value of **_database_PDB_tvect.id** must uniquely identify a record in the DATABASE_PDB_TVECT list. Note that this item need not be a number; it can be any unique identifier.
**[database_PDB_tvect]**

**_database_PDB_tvect.vector[1]** (*float*)
The [1] element of the PDB TVECT vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_tvect]**

**_database_PDB_tvect.vector[2]** (*float*)
The [2] element of the PDB TVECT vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_tvect]**

**_database_PDB_tvect.vector[3]** (*float*)
The [3] element of the PDB TVECT vector.
Where no value is given, the assumed value is '0.0'. **[database_PDB_tvect]**

## DIFFRN

Data items in the DIFFRN category record details about the diffraction data and their measurement.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn.id                          'Set1'
_diffrn.ambient_temp                 293(3)
_diffrn.ambient_environment
; Mother liquor from the reservoir of the vapor diffusion
  experiment, mounted in room air
;
_diffrn.crystal_support
; 0.7 mm glass capillary, sealed with dental wax
;
_diffrn.crystal_treatment
; Equilibrated in rotating anode radiation enclosure for
  18 hours prior to beginning of data collection
;
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [(1991). Acta Cryst. C**47**, 2276–2277].*

```
_diffrn.id              'd1'
_diffrn.details
; \q scan width (1.0 + 0.14tan\q)\%, \q scan rate 1.2\% per
   min. Background counts for 5 sec on each side every scan.
;
_diffrn.ambient_temp     293
```

**_diffrn.ambient_environment** (*line*)
***_diffrn_ambient_environment*** (*cif_core.dic 2.0.1*)
The gas or liquid surrounding the sample, if not air.
**[diffrn]**

**_diffrn.ambient_pressure** (*float, su*)
***_diffrn_ambient_pressure*** (*cif_core.dic 2.3*)
The mean hydrostatic pressure in kilopascals at which the intensities were measured.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_pressure_esd** (associated esd). **[diffrn]**

**_diffrn.ambient_pressure_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_diffrn.ambient_pressure**.
Related item: **_diffrn.ambient_pressure** (associated value). **[diffrn]**

**_diffrn.ambient_pressure_gt** (*float*)
***_diffrn_ambient_pressure_gt*** (*cif_core.dic 2.3*)
The mean hydrostatic pressure in kilopascals above which the intensities were measured. **_diffrn.ambient_pressure_gt** and **_diffrn.ambient_pressure_lt** allow a pressure range to be given. **_diffrn.ambient_pressure** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_pressure** (alternate). **[diffrn]**

**_diffrn.ambient_pressure_lt** (*float*)
***_diffrn_ambient_pressure_lt*** (*cif_core.dic 2.3*)
The mean hydrostatic pressure in kilopascals below which the intensities were measured. **_diffrn.ambient_pressure_gt** and **_diffrn.ambient_pressure_lt** allow a pressure range to be given. **_diffrn.ambient_pressure** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_pressure** (alternate). **[diffrn]**

**_diffrn.ambient_temp** (*float, su*)
***_diffrn_ambient_temperature*** (*cif_core.dic 2.0.1*)
The mean temperature in kelvins at which the intensities were measured.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_temp_esd** (associated esd). **[diffrn]**

**_diffrn.ambient_temp_details** (*text*)
A description of special aspects of temperature control during data collection.
**[diffrn]**

**_diffrn.ambient_temp_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_diffrn.ambient_temp**.
Related item: **_diffrn.ambient_temp** (associated value). **[diffrn]**

**_diffrn.ambient_temp_gt** (*float*)
***_diffrn_ambient_temperature_gt*** (*cif_core.dic 2.3*)
The mean temperature in kelvins above which the intensities were measured. **_diffrn.ambient_temp_gt** and **_diffrn.ambient_temp_lt** allow a range of temperatures to be given. **_diffrn.ambient_temp** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_temp** (alternate). **[diffrn]**

**_diffrn.ambient_temp_lt** (*float*)
***_diffrn_ambient_temperature_lt*** (*cif_core.dic 2.3*)
The mean temperature in kelvins below which the intensities were measured. **_diffrn.ambient_temp_gt** and **_diffrn.ambient_temp_lt** allow a range of temperatures to be given. **_diffrn.ambient_temp** should always be used in preference to these two items whenever possible.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn.ambient_temp** (alternate). **[diffrn]**

* **_diffrn.crystal_id**
***_diffrn_refln_crystal_id*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_exptl_crystal.id** in the EXPTL_CRYSTAL category.

**_diffrn.crystal_support** (*text*)
The physical device used to support the crystal during data collection.
Examples: 'glass capillary', 'quartz capillary', 'fiber', 'metal loop'.
**[diffrn]**

**_diffrn.crystal_treatment** (*text*)
***_diffrn_crystal_treatment*** (*cif_core.dic 2.0.1*)
Remarks about how the crystal was treated prior to intensity measurement. Particularly relevant when intensities were measured at low temperature.
Examples: 'equilibrated in hutch for 24 hours',
'flash frozen in liquid nitrogen',
'slow cooled with direct air stream'. **[diffrn]**

**_diffrn.details** (*text*)
***_diffrn_special_details*** (*cif_core.dic 2.0.1*)
Special details of the diffraction measurement process. Should include information about source instability, crystal motion, degradation and so on.
**[diffrn]**

* **_diffrn.id** (*code*)
This data item uniquely identifies a set of diffraction data.
*The following item(s) have an equivalent role in their respective categories:*
***_diffrn_detector.diffrn_id***,
***_diffrn_measurement.diffrn_id***,
***_diffrn_orient_matrix.diffrn_id***,
***_diffrn_orient_refln.diffrn_id***,
***_diffrn_radiation.diffrn_id***,
***_diffrn_refln.diffrn_id***,
***_diffrn_reflns.diffrn_id***,
***_diffrn_source.diffrn_id***,
***_diffrn_standard_refln.diffrn_id***,
***_diffrn_standards.diffrn_id***. **[diffrn]**

## DIFFRN_ATTENUATOR

Data items in the DIFFRN_ATTENUATOR category record details about the diffraction attenuator scales employed.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_attenuator.code**

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276-2277].*

```
_diffrn_attenuator.code       1
_diffrn_attenuator.scale      16.976
```

* **_diffrn_attenuator.code** (*code*)
***_diffrn_attenuator_code*** (*cif_core.dic 2.0.1*)
A code associated with a particular attenuator setting. This code is referenced by the **_diffrn_refln.attenuator_code** which is stored with the diffraction data. See **_diffrn_attenuator.scale**.
**[diffrn_attenuator]**

**_diffrn_attenuator.material** (*text*)
***_diffrn_attenuator_material*** (*cif_core.dic 2.3*)
Material from which the attenuator is made.
**[diffrn_attenuator]**

### _diffrn_attenuator.scale (*float*)

***_diffrn_attenuator_scale*** (*cif_core.dic 2.0.1*)

The scale factor applied when an intensity measurement is reduced by an attenuator identified by **_diffrn_attenuator.code**. The measured intensity must be multiplied by this scale to convert it to the same scale as unattenuated intensities.

The permitted range is $[1.0, \infty)$. **[diffrn_attenuator]**

## DIFFRN_DETECTOR

Data items in the DIFFRN_DETECTOR category describe the detector used to measure the scattered radiation, including any analyser and post-sample collimation.

Category group(s): **inclusive_group**
**diffrn_group**

Category key(s): **_diffrn_detector.diffrn_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn_detector.diffrn_id            'd1'
_diffrn_detector.detector             'multiwire'
_diffrn_detector.type                 'Siemens'
```

### _diffrn_detector.area_resol_mean (*float*)

***_diffrn_detector_area_resol_mean*** (*cif_core.dic 2.3*)

The resolution of an area detector, in pixels $mm^{-1}$.

The permitted range is $[0.0, \infty)$. **[diffrn_detector]**

### _diffrn_detector.details (*text*)

***_diffrn_detector_details*** (*cif_core.dic 2.0.1*)

A description of special aspects of the radiation detector.

**[diffrn_detector]**

### _diffrn_detector.detector (*text*)

***_diffrn_radiation_detector*** (*cifdic.c91 1.0*)
***_diffrn_detector*** (*cif_core.dic 2.0*)

The general class of the radiation detector.

Examples: 'photographic film', 'scintillation counter', 'CCD plate', 'BF~3~ counter'. **[diffrn_detector]**

### *_diffrn_detector.diffrn_id

This data item is a pointer to **_diffrn.id** in the DIFFRN category.

### _diffrn_detector.dtime (*float*)

***_diffrn_detector_dtime*** (*cif_core.dic 2.3*)

The deadtime in microseconds of the detector used to measure the diffraction intensities.

The permitted range is $[0.0, \infty)$. **[diffrn_detector]**

### _diffrn_detector.type (*text*)

***_diffrn_detector_type*** (*cif_core.dic 2.0.1*)

The make, model or name of the detector device used.

**[diffrn_detector]**

## DIFFRN_MEASUREMENT

Data items in the DIFFRN_MEASUREMENT category record details about the device used to orient and/or position the crystal during data measurement and the manner in which the diffraction data were measured.

Category group(s): **inclusive_group**
**diffrn_group**

Category key(s): **_diffrn_measurement.diffrn_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn_measurement.diffrn_id         'd1'
_diffrn_measurement.device            '3-circle camera'
_diffrn_measurement.device_type       'Supper model x'
_diffrn_measurement.device_details    'none'
_diffrn_measurement.method            'omega scan'
_diffrn_measurement.details
; 440 frames, 0.20 degrees, 150 sec, detector distance 12 cm,
  detector angle 22.5 degrees
;
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
_diffrn_measurement.diffrn_id      's1'
_diffrn_measurement.device_type
     'Philips PW1100/20 diffractometer'
_diffrn_measurement.method         \q/2\q
```

### _diffrn_measurement.details (*text*)

***_diffrn_measurement_details*** (*cif_core.dic 2.0.1*)

A description of special aspects of the intensity measurement.

Example:

```
; 440 frames, 0.20 degrees, 150 sec, detector
  distance 12 cm, detector angle 22.5 degrees
;
```

**[diffrn_measurement]**

### _diffrn_measurement.device (*text*)

***_diffrn_measurement_device*** (*cif_core.dic 2.0.1*)

The general class of goniometer or device used to support and orient the specimen.

Examples: '3-circle camera', '4-circle camera', 'kappa-geometry camera', 'oscillation camera', 'precession camera'.

**[diffrn_measurement]**

### _diffrn_measurement.device_details (*text*)

***_diffrn_measurement_device_details*** (*cif_core.dic 2.0.1*)

A description of special aspects of the device used to measure the diffraction intensities.

Example:

```
; commercial goniometer modified locally to
  allow for 90\% \t arc
;
```

**[diffrn_measurement]**

### _diffrn_measurement.device_type (*text*)

***_diffrn_measurement_device_type*** (*cif_core.dic 2.0.1*)

The make, model or name of the measurement device (goniometer) used.

Examples: 'Supper model q', 'Huber model r', 'Enraf-Nonius model s', 'homemade'. **[diffrn_measurement]**

### *_diffrn_measurement.diffrn_id

This data item is a pointer to **_diffrn.id** in the DIFFRN category.

### _diffrn_measurement.method (*text*)

***_diffrn_measurement_method*** (*cif_core.dic 2.0.1*)

Method used to measure intensities.

Example: 'profile data from theta/2theta scans'.

**[diffrn_measurement]**

**_diffrn_measurement.specimen_support** (*text*)
***_diffrn_measurement_specimen_support*** (*cif_core.dic 2.0.1*)
The physical device used to support the crystal during data collection.
Examples: 'glass capillary', 'quartz capillary', 'fiber', 'metal loop'.
**[diffrn_measurement]**

## DIFFRN_ORIENT_MATRIX

Data items in the DIFFRN_ORIENT_MATRIX category record details about the orientation matrix used in the measurement of the diffraction data.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_orient_matrix.diffrn_id**

*Example 1 – based on CAD-4 diffractometer data obtained for Yb(S-$C_5H_4N$)$_2$-(THF)$_4$.*

```
_diffrn_orient_matrix.diffrn_id   set1
_diffrn_orient_matrix.type
; reciprocal axis matrix, multiplies hkl vector to generate
  diffractometer xyz vector and diffractometer angles
;
_diffrn_orient_matrix.UB[1][1]    -0.071479
_diffrn_orient_matrix.UB[1][2]     0.020208
_diffrn_orient_matrix.UB[1][3]     0.039076
_diffrn_orient_matrix.UB[2][1]     0.035372
_diffrn_orient_matrix.UB[2][2]     0.056209
_diffrn_orient_matrix.UB[2][3]     0.078324
_diffrn_orient_matrix.UB[3][1]    -0.007470
_diffrn_orient_matrix.UB[3][2]     0.067854
_diffrn_orient_matrix.UB[3][3]    -0.017832
```

* **_diffrn_orient_matrix.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

**_diffrn_orient_matrix.type** (*text*)
***_diffrn_orient_matrix_type*** (*cif_core.dic 2.0.1*)
A description of the orientation matrix type and how it should be applied to define the orientation of the crystal precisely with respect to the diffractometer axes.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[1][1]** (*float*)
***_diffrn_orient_matrix_UB_11*** (*cif_core.dic 2.0.1*)
The [1][1] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[1][2]** (*float*)
***_diffrn_orient_matrix_UB_12*** (*cif_core.dic 2.0.1*)
The [1][2] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[1][3]** (*float*)
***_diffrn_orient_matrix_UB_13*** (*cif_core.dic 2.0.1*)
The [1][3] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[2][1]** (*float*)
***_diffrn_orient_matrix_UB_21*** (*cif_core.dic 2.0.1*)
The [2][1] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[2][2]** (*float*)
***_diffrn_orient_matrix_UB_22*** (*cif_core.dic 2.0.1*)
The [2][2] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[2][3]** (*float*)
***_diffrn_orient_matrix_UB_23*** (*cif_core.dic 2.0.1*)
The [2][3] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[3][1]** (*float*)
***_diffrn_orient_matrix_UB_31*** (*cif_core.dic 2.0.1*)
The [3][1] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[3][2]** (*float*)
***_diffrn_orient_matrix_UB_32*** (*cif_core.dic 2.0.1*)
The [3][2] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

**_diffrn_orient_matrix.UB[3][3]** (*float*)
***_diffrn_orient_matrix_UB_33*** (*cif_core.dic 2.0.1*)
The [3][3] element of the 3 × 3 matrix that defines the dimensions of the reciprocal cell and its orientation with respect to the local diffractometer axes. See also **_diffrn_orient_matrix.type**.
**[diffrn_orient_matrix]**

## DIFFRN_ORIENT_REFLN

Data items in the DIFFRN_ORIENT_REFLN category record details about the reflections that define the orientation matrix used in the measurement of the diffraction intensities.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_orient_refln.diffrn_id**
**_diffrn_orient_refln.index_h**
**_diffrn_orient_refln.index_k**
**_diffrn_orient_refln.index_l**

*Example 1 – based on CAD-4 diffractometer data obtained for Yb(S-$C_5H_4N$)$_2$-(THF)$_4$.*

```
_diffrn_orient_refln.diffrn_id    myset1
_diffrn_orient_refln.index_h      2
_diffrn_orient_refln.index_k      0
_diffrn_orient_refln.index_l      2
_diffrn_orient_refln.angle_chi    -28.45
_diffrn_orient_refln.angle_kappa  -11.32
_diffrn_orient_refln.angle_omega  5.33
_diffrn_orient_refln.angle_phi    101.78
_diffrn_orient_refln.angle_psi    0.00
_diffrn_orient_refln.angle_theta  10.66
# ... data abbreviated  ...
```

**_diffrn_orient_refln.angle_chi** (*float*)
***_diffrn_orient_refln_angle_chi*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\chi$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

**_diffrn_orient_refln.angle_kappa** (*float*)
***_diffrn_orient_refln_angle_kappa*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\kappa$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

**_diffrn_orient_refln.angle_omega** (*float*)
***_diffrn_orient_refln_angle_omega*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\omega$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

**_diffrn_orient_refln.angle_phi** (*float*)
***_diffrn_orient_refln_angle_phi*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\varphi$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

**_diffrn_orient_refln.angle_psi** (*float*)
***_diffrn_orient_refln_angle_psi*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\psi$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

**_diffrn_orient_refln.angle_theta** (*float*)
***_diffrn_orient_refln_angle_theta*** (*cif_core.dic 2.0.1*)
Diffractometer angle $\theta$ of a reflection used to define the orientation matrix in degrees. See **_diffrn_orient_matrix.UB**[][] and the Miller indices in the DIFFRN_ORIENT_REFLN category.
**[diffrn_orient_refln]**

***_diffrn_orient_refln.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

***_diffrn_orient_refln.index_h** (*int*)
***_diffrn_orient_refln_index_h*** (*cif_core.dic 2.0.1*)
Miller index *h* of a reflection used to define the orientation matrix.
**[diffrn_orient_refln]**

***_diffrn_orient_refln.index_k** (*int*)
***_diffrn_orient_refln_index_k*** (*cif_core.dic 2.0.1*)
Miller index *k* of a reflection used to define the orientation matrix.
**[diffrn_orient_refln]**

***_diffrn_orient_refln.index_l** (*int*)
***_diffrn_orient_refln_index_l*** (*cif_core.dic 2.0.1*)
Miller index *l* of a reflection used to define the orientation matrix.
**[diffrn_orient_refln]**

## DIFFRN_RADIATION

Data items in the DIFFRN_RADIATION category describe the radiation used in measuring the diffraction intensities, its collimation and monochromatization before the sample. Post-sample treatment of the beam is described by data items in the DIFFRN_DETECTOR category.

Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_radiation.diffrn_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn_radiation.diffrn_id          'set1'

_diffrn_radiation.collimation        '0.3 mm double pinhole'
_diffrn_radiation.monochromator      'graphite'
_diffrn_radiation.type               'Cu K\a'
_diffrn_radiation.wavelength_id       1
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
_diffrn_radiation.wavelength_id   1
_diffrn_radiation.type            'Cu K\a'
_diffrn_radiation.monochromator   'graphite'
```

**_diffrn_radiation.collimation** (*text*)
***_diffrn_radiation_collimation*** (*cif_core.dic 2.0.1*)
The collimation or focusing applied to the radiation.
Examples: '`0.3 mm double-pinhole`', '`0.5 mm`', '`focusing mirrors`'.
**[diffrn_radiation]**

***_diffrn_radiation.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

**_diffrn_radiation.filter_edge** (*float*)
***_diffrn_radiation_filter_edge*** (*cif_core.dic 2.0.1*)
Absorption edge in ångströms of the radiation filter used.
The permitted range is $[0.0, \infty)$. **[diffrn_radiation]**

**_diffrn_radiation.inhomogeneity** (*float*)
***_diffrn_radiation_inhomogeneity*** (*cif_core.dic 2.0.1*)
Half-width in millimetres of the incident beam in the direction perpendicular to the diffraction plane.
The permitted range is $[0.0, \infty)$. **[diffrn_radiation]**

**_diffrn_radiation.monochromator** (*text*)
***_diffrn_radiation_monochromator*** (*cif_core.dic 2.0.1*)
The method used to obtain monochromatic radiation. If a monochromator crystal is used, the material and the indices of the Bragg reflection are specified.
Examples: '`Zr filter`', '`Ge 220`', '`none`', '`equatorial mounted graphite`'.
**[diffrn_radiation]**

**_diffrn_radiation.polarisn_norm** (*float*)
***_diffrn_radiation_polarisn_norm*** (*cif_core.dic 2.0.1*)
The angle in degrees, as viewed from the specimen, between the perpendicular component of the polarization and the diffraction plane. See **_diffrn_radiation.polarisn_ratio**.
The permitted range is $[0.0, \infty)$. **[diffrn_radiation]**

**_diffrn_radiation.polarisn_ratio** (*float*)
***_diffrn_radiation_polarisn_ratio*** (*cif_core.dic 2.0.1*)
Polarization ratio of the diffraction beam incident on the crystal. This is the ratio of the perpendicularly polarized to the parallel-polarized component of the radiation. The perpendicular component forms an angle of **_diffrn_radiation.polarisn_norm** to the normal to the diffraction plane of the sample (*i.e.* the plane containing the incident and reflected beams).
The permitted range is $[0.0, \infty)$. **[diffrn_radiation]**

### _diffrn_radiation.probe (*line*)

_diffrn_radiation_probe (*cif_core.dic 2.0.1*)

The nature of the radiation used (*i.e.* the name of the subatomic particle or the region of the electromagnetic spectrum). It is strongly recommended that this information be given, so that the probe radiation can be simply determined.

The data value must be one of the following:

- x-ray
- neutron
- electron
- gamma

**[diffrn_radiation]**

### _diffrn_radiation.type (*line*)

_diffrn_radiation_type (*cif_core.dic 2.0.1*)

The nature of the radiation. This is typically a description of the X-ray wavelength in Siegbahn notation.

Examples: 'CuK\a', 'Cu K\a~1~', 'Cu K-L~2,3~', 'white-beam'.

**[diffrn_radiation]**

### *_diffrn_radiation.wavelength_id

This data item is a pointer to **_diffrn_radiation_wavelength.id** in the DIFFRN_RADIATION_WAVELENGTH category.

### _diffrn_radiation.xray_symbol (*line*)

_diffrn_radiation_xray_symbol (*cif_core.dic 2.0.1*)

The IUPAC symbol for the X-ray wavelength for the probe radiation.

The data value must be one of the following:

| | |
|---|---|
| K-L~3~ | $K\alpha_1$ in older Siegbahn notation |
| K-L~2~ | $K\alpha_2$ in older Siegbahn notation |
| K-M~3~ | $K\beta$ in older Siegbahn notation |
| K-L~2,3~ | use where *K*-$L_3$ and *K*-$L_2$ are not resolved |

**[diffrn_radiation]**

## DIFFRN_RADIATION_WAVELENGTH

Data items in the DIFFRN_RADIATION_WAVELENGTH category describe the wavelength of the radiation used to measure the diffraction intensities. Items may be looped to identify and assign weights to distinct components of a polychromatic beam.

Category group(s): **inclusive_group**, **diffrn_group**

Category key(s): **_diffrn_radiation_wavelength.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn_radiation_wavelength.id              1
_diffrn_radiation_wavelength.wavelength      1.54
_diffrn_radiation_wavelength.wt              1.0
```

### *_diffrn_radiation_wavelength.id (*code*)

_diffrn_radiation_wavelength_id (*cif_core.dic 2.0.1*)

The code identifying each value of **_diffrn_radiation_wavelength.wavelength**. Items in the DIFFRN_RADIATION_WAVELENGTH category are looped when multiple wavelengths are used. This code is used to link with the DIFFRN_REFLN category. The **_diffrn_refln.wavelength_id** codes must match one of the codes defined in this category.

*The following item(s) have an equivalent role in their respective categories:*

**_diffrn_radiation.wavelength_id**,

**_diffrn_refln.wavelength_id**,

**_refln.wavelength_id**.

Examples: 'x1', 'x2', 'neut'. **[diffrn_radiation_wavelength]**

### *_diffrn_radiation_wavelength.wavelength (*float*)

_diffrn_radiation_wavelength (*cif_core.dic 2.0.1*)

The radiation wavelength in ångströms.

The permitted range is $[0.0, \infty)$. **[diffrn_radiation_wavelength]**

### _diffrn_radiation_wavelength.wt (*float*)

_diffrn_radiation_wavelength_wt (*cif_core.dic 2.0.1*)

The relative weight of a wavelength identified by the code **_diffrn_radiation_wavelength.id** in the list of wavelengths.

The permitted range is [0.0, 1.0]. Where no value is given, the assumed value is '1.0'.

**[diffrn_radiation_wavelength]**

## DIFFRN_REFLN

Data items in the DIFFRN_REFLN category record details about the intensities in the diffraction data set identified by **_diffrn_refln.diffrn_id**. The DIFFRN_REFLN data items refer to individual intensity measurements and must be included in looped lists. The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements in the particular diffraction data set identified by **_diffrn_reflns.diffrn_id**.

Category group(s): **inclusive_group**, **diffrn_group**

Category key(s): **_diffrn_refln.diffrn_id**, **_diffrn_refln.id**

*Example 1 – based on CAD-4 diffractometer data obtained for Yb(S-$C_5H_4N$)$_2$-(THF)$_4$ for data set 'set1' reflection 1102.*

```
_diffrn_refln.diffrn_id            set1
_diffrn_refln.id                   1102
_diffrn_refln.wavelength_id        Cu1fixed
_diffrn_refln.angle_chi            32.21
_diffrn_refln.angle_kappa          20.12
_diffrn_refln.angle_omega          11.54
_diffrn_refln.angle_phi            176.02
_diffrn_refln.angle_psi            0.00
_diffrn_refln.angle_theta          23.08
_diffrn_refln.attenuator_code      'Ni.005'
_diffrn_refln.counts_bg_1          22
_diffrn_refln.counts_bg_2          25
_diffrn_refln.counts_net           3450
_diffrn_refln.counts_peak          321
_diffrn_refln.counts_total         3499
_diffrn_refln.detect_slit_horiz    0.04
_diffrn_refln.detect_slit_vert     0.02
_diffrn_refln.elapsed_time         1.00
_diffrn_refln.index_h              4
_diffrn_refln.index_k              0
_diffrn_refln.index_l              2
_diffrn_refln.intensity_net        202.56
_diffrn_refln.intensity_sigma      2.18
_diffrn_refln.scale_group_code     A24
_diffrn_refln.scan_mode            om
_diffrn_refln.scan_mode_backgd     mo
_diffrn_refln.scan_rate            1.2
_diffrn_refln.scan_time_backgd     900.00
_diffrn_refln.scan_width           1.0
_diffrn_refln.sint_over_lambda     0.25426
_diffrn_refln.standard_code        1
_diffrn_refln.wavelength           1.54184
```

### _diffrn_refln.angle_chi (*float*)

_diffrn_refln_angle_chi (*cif_core.dic 2.0.1*)

The diffractometer angle $\chi$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.

**[diffrn_refln]**

### _diffrn_refln.angle_kappa (*float*)

_diffrn_refln_angle_kappa (*cif_core.dic 2.0.1*)

The diffractometer angle $\kappa$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.

**[diffrn_refln]**

**_diffrn_refln.angle_omega** (*float*)
***_diffrn_refln_angle_omega*** (*cif_core.dic 2.0.1*)
The diffractometer angle $\omega$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.
**[diffrn_refln]**

**_diffrn_refln.angle_phi** (*float*)
***_diffrn_refln_angle_phi*** (*cif_core.dic 2.0.1*)
The diffractometer angle $\varphi$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.
**[diffrn_refln]**

**_diffrn_refln.angle_psi** (*float*)
***_diffrn_refln_angle_psi*** (*cif_core.dic 2.0.1*)
The diffractometer angle $\psi$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.
**[diffrn_refln]**

**_diffrn_refln.angle_theta** (*float*)
***_diffrn_refln_angle_theta*** (*cif_core.dic 2.0.1*)
The diffractometer angle $\theta$ of a reflection in degrees. This angle corresponds to the specified orientation matrix and the original measured cell before any subsequent cell transformations.
**[diffrn_refln]**

**_diffrn_refln.attenuator_code**
***_diffrn_refln_attenuator_code*** (*cif_core.dic 2.0.1*)
The code identifying the attenuator setting for this reflection. This code must match one of the **_diffrn_attenuator.code** values.

**_diffrn_refln.class_code** (*code*)
***_diffrn_refln_class_code*** (*cif_core.dic 2.3*)
The code identifying the class to which this reflection has been assigned. This code must match a value of **_diffrn_reflns.class_code**. Reflections may be grouped into classes for a variety of purposes. For example, for modulated structures each reflection class may be defined by the number $m = \sum |m_i|$, where the $m_i$ are the integer coefficients that, in addition to $h, k, l$, index the corresponding diffraction vector in the basis defined for the reciprocal lattice.
**[diffrn_refln]**

**_diffrn_refln.counts_bg_1** (*int*)
***_diffrn_refln_counts_bg_1*** (*cif_core.dic 2.0.1*)
The diffractometer counts for the measurement of the background before the peak.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.counts_bg_2** (*int*)
***_diffrn_refln_counts_bg_2*** (*cif_core.dic 2.0.1*)
The diffractometer counts for the measurement of the background after the peak.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.counts_net** (*int*)
***_diffrn_refln_counts_net*** (*cif_core.dic 2.0.1*)
The diffractometer counts for the measurement of net counts after background removal.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.counts_peak** (*int*)
***_diffrn_refln_counts_peak*** (*cif_core.dic 2.0.1*)
The diffractometer counts for the measurement of counts for the peak scan or position.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.counts_total** (*int*)
***_diffrn_refln_counts_total*** (*cif_core.dic 2.0.1*)
The diffractometer counts for the measurement of total counts (background plus peak).
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.detect_slit_horiz** (*float*)
***_diffrn_refln_detect_slit_horiz*** (*cif_core.dic 2.0.1*)
Total slit aperture in degrees in the diffraction plane.
The permitted range is $[0.0, 90.0]$. **[diffrn_refln]**

**_diffrn_refln.detect_slit_vert** (*float*)
***_diffrn_refln_detect_slit_vert*** (*cif_core.dic 2.0.1*)
Total slit aperture in degrees perpendicular to the diffraction plane.
The permitted range is $[0.0, 90.0]$. **[diffrn_refln]**

* **_diffrn_refln.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

**_diffrn_refln.elapsed_time** (*float*)
***_diffrn_refln_elapsed_time*** (*cif_core.dic 2.0.1*)
Elapsed time in minutes from the start of the diffraction experiment to the measurement of this intensity.
The permitted range is $[0.0, \infty)$. **[diffrn_refln]**

* **_diffrn_refln.id** (*code*)
The value of **_diffrn_refln.id** must uniquely identify the reflection in the data set identified by the item **_diffrn_refln.diffrn_id**. Note that this item need not be a number; it can be any unique identifier.
**[diffrn_refln]**

* **_diffrn_refln.index_h** (*int*)
***_diffrn_refln_index_h*** (*cif_core.dic 2.0.1*)
Miller index $h$ of a reflection. The values of the Miller indices in the DIFFRN_REFLN category need not match the values of the Miller indices in the REFLN category if a transformation of the original measured cell has taken place. Details of the cell transformation are given in **_diffrn_reflns.reduction_process**. See also **_diffrn_reflns.transf_matrix**[][].
**[diffrn_refln]**

* **_diffrn_refln.index_k** (*int*)
***_diffrn_refln_index_k*** (*cif_core.dic 2.0.1*)
Miller index $k$ of a reflection. The values of the Miller indices in the DIFFRN_REFLN category need not match the values of the Miller indices in the REFLN category if a transformation of the original measured cell has taken place. Details of the cell transformation are given in **_diffrn_reflns.reduction_process**. See also **_diffrn_reflns.transf_matrix**[][].
**[diffrn_refln]**

* **_diffrn_refln.index_l** (*int*)
***_diffrn_refln_index_l*** (*cif_core.dic 2.0.1*)
Miller index $l$ of a reflection. The values of the Miller indices in the DIFFRN_REFLN category need not match the values of the Miller indices in the REFLN category if a transformation of the original measured cell has taken place. Details of the cell transformation are given in **_diffrn_reflns.reduction_process**. See also **_diffrn_reflns.transf_matrix**[][].
**[diffrn_refln]**

**_diffrn_refln.intensity_net** (*float*)
***_diffrn_refln_intensity_net*** (*cif_core.dic 2.0.1*)
Net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.intensity_sigma** (*float*)
***_diffrn_refln_intensity_sigma*** (*cif_core.dic 2.0.1*)
Standard uncertainty (estimated standard deviation) of the intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.
The permitted range is $[0, \infty)$. **[diffrn_refln]**

**_diffrn_refln.intensity_u** (*float*)
***_diffrn_refln_intensity_u*** (*cif_core.dic 2.3*)
Standard uncertainty of the net intensity calculated from the diffraction counts after the attenuator and standard scales have been applied.
The permitted range is $[0.0, \infty)$.
Related item: **_diffrn_refln.intensity_sigma** (alternate). **[diffrn_refln]**

***_diffrn_refln.scale_group_code**
***_diffrn_refln_scale_group_code*** (*cif_core.dic 2.0.1*)
The code identifying the scale applying to this reflection. This data item is a pointer to **_diffrn_scale_group.code** in the DIFFRN_SCALE_GROUP category.

**_diffrn_refln.scan_mode** (*ucode*)
***_diffrn_refln_scan_mode*** (*cif_core.dic 2.0.1*)
The code identifying the mode of scanning for measurements using a diffractometer. See **_diffrn_refln.scan_width** and **_diffrn_refln.scan_mode_backgd**.
The data value must be one of the following:

| | |
|---|---|
| om | $\omega$ scan |
| ot | $\omega/2\theta$ scan |
| q | $Q$ scans (arbitrary reciprocal directions) |

**[diffrn_refln]**

**_diffrn_refln.scan_mode_backgd** (*ucode*)
***_diffrn_refln_scan_mode_backgd*** (*cif_core.dic 2.0.1*)
The code identifying the mode of scanning a reflection to measure the background intensity.
The data value must be one of the following:

| | |
|---|---|
| st | stationary counter background |
| mo | moving counter background |

**[diffrn_refln]**

**_diffrn_refln.scan_rate** (*float*)
***_diffrn_refln_scan_rate*** (*cif_core.dic 2.0.1*)
The rate of scanning a reflection in degrees per minute to measure the intensity.
**[diffrn_refln]**

**_diffrn_refln.scan_time_backgd** (*float*)
***_diffrn_refln_scan_time_backgd*** (*cif_core.dic 2.0.1*)
The time spent measuring each background in seconds.
**[diffrn_refln]**

**_diffrn_refln.scan_width** (*float*)
***_diffrn_refln_scan_width*** (*cif_core.dic 2.0.1*)
The scan width in degrees of the scan mode defined by the code **_diffrn_refln.scan_mode**.
The permitted range is $[0.0, 90.0]$. **[diffrn_refln]**

**_diffrn_refln.sint_over_lambda** (*float*)
***_diffrn_refln_sint/lambda*** (*cif_core.dic 2.0.1*)
The $(\sin\theta)/\lambda$ value in reciprocal ångströms for this reflection.
The permitted range is $[0.0, \infty)$. **[diffrn_refln]**

***_diffrn_refln.standard_code**
***_diffrn_refln_standard_code*** (*cif_core.dic 2.0.1*)
The code identifying that this reflection was measured as a standard intensity. This data item is a pointer to **_diffrn_standard_refln.code** in the DIFFRN_STANDARD_REFLN category.

**_diffrn_refln.wavelength** (*float*)
***_diffrn_refln_wavelength*** (*cif_core.dic 2.0.1*)
The mean wavelength in ångströms of the radiation used to measure the intensity of this reflection. This is an important parameter for data collected using energy-dispersive detectors or the Laue method.
The permitted range is $[0.0, \infty)$. **[diffrn_refln]**

***_diffrn_refln.wavelength_id**
***_diffrn_refln_wavelength_id*** (*cif_core.dic 2.0.1*)
This data item is a pointer to **_diffrn_radiation.wavelength_id** in the DIFFRN_RADIATION category.

## DIFFRN_REFLNS

Data items in the DIFFRN_REFLNS category record details about the set of intensities measured in the diffraction experiment. The DIFFRN_REFLN data items refer to individual intensity measurements and must be included in looped lists. The DIFFRN_REFLNS data items specify the parameters that apply to all intensity measurements in a diffraction data set.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_reflns.diffrn_id**

**_diffrn_reflns.av_R_equivalents** (*float*)
***_diffrn_reflns_av_R_equivalents*** (*cif_core.dic 2.0.1*)
The residual $[\sum \mathrm{av}|\Delta(I)| / \sum |\mathrm{av}(I)|]$ for symmetry-equivalent reflections used to calculate the average intensity $\mathrm{av}(I)$. The $\mathrm{av}|\Delta(I)|$ term is the average absolute difference between $\mathrm{av}(I)$ and the individual symmetry-equivalent intensities.
The permitted range is $[0.0, \infty)$. **[diffrn_reflns]**

**_diffrn_reflns.av_sigmaI_over_netI** (*float*)
***_diffrn_reflns_av_sigmaI/netI*** (*cif_core.dic 2.0.1*)
Measure $[\sum |\sigma(\mathrm{net}\ I)| / \sum |\mathrm{net}\ I|]$ for all measured reflections.
The permitted range is $[0.0, \infty)$. **[diffrn_reflns]**

**_diffrn_reflns.av_unetI/netI** (*float*)
***_diffrn_reflns_av_unetI/netI*** (*cif_core.dic 2.3*)
Measure $[\sum |u(\mathrm{net}\ I)| / \sum |\mathrm{net}\ I|]$ for all measured reflections.
The permitted range is $[0.0, \infty)$. **[diffrn_reflns]**

***_diffrn_reflns.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

**_diffrn_reflns.limit_h_max** (*int*)
***_diffrn_reflns_limit_h_max*** (*cif_core.dic 2.0.1*)
The maximum value of the Miller index $h$ for the reflection data specified by **_diffrn_refln.index_h**.
**[diffrn_reflns]**

**_diffrn_reflns.limit_h_min** (*int*)
***_diffrn_reflns_limit_h_min*** (*cif_core.dic 2.0.1*)
The minimum value of the Miller index $h$ for the reflection data specified by **_diffrn_refln.index_h**.
**[diffrn_reflns]**

**_diffrn_reflns.limit_k_max** (*int*)
***_diffrn_reflns_limit_k_max*** (*cif_core.dic 2.0.1*)
The maximum value of the Miller index $k$ for the reflection data specified by **_diffrn_refln.index_k**.
**[diffrn_reflns]**

**_diffrn_reflns.limit_k_min** (*int*)
***_diffrn_reflns_limit_k_min*** (*cif_core.dic 2.0.1*)
The minimum value of the Miller index $k$ for the reflection data specified by **_diffrn_refln.index_k**.
**[diffrn_reflns]**

**_diffrn_reflns.limit_l_max** (*int*)
***_diffrn_reflns_limit_l_max*** (*cif_core.dic 2.0.1*)
The maximum value of the Miller index $l$ for the reflection data specified by **_diffrn_refln.index_l**.
**[diffrn_reflns]**

**_diffrn_reflns.limit_l_min** (*int*)
***_diffrn_reflns_limit_l_min*** (*cif_core.dic 2.0.1*)
The minimum value of the Miller index $l$ for the reflection data specified by **_diffrn_refln.index_l**.
**[diffrn_reflns]**

**_diffrn_reflns.number** (*int*)
***_diffrn_reflns_number*** (*cif_core.dic 2.0.1*)
The total number of measured intensities, excluding reflections that are classified as systematically absent.
The permitted range is $[0, \infty)$. **[diffrn_reflns]**

**_diffrn_reflns.reduction_process** (*text*)
***_diffrn_reflns_reduction_process*** (*cif_core.dic 2.0.1*)
A description of the process used to reduce the intensity data into structure-factor magnitudes.
Example: 'data averaged using Fisher test'. **[diffrn_reflns]**

**_diffrn_reflns.theta_max** (*float*)
***_diffrn_reflns_theta_max*** (*cif_core.dic 2.0.1*)
Maximum $\theta$ angle in degrees for the measured diffraction intensities.
The permitted range is $[0.0, 90.0]$. **[diffrn_reflns]**

**_diffrn_reflns.theta_min** (*float*)
***_diffrn_reflns_theta_min*** (*cif_core.dic 2.0.1*)
Minimum $\theta$ angle in degrees for the measured diffraction intensities.
The permitted range is $[0.0, 90.0]$. **[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[1][1]** (*float*)
***_diffrn_reflns_transf_matrix_11*** (*cif_core.dic 2.0.1*)
The [1][1] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[1][2]** (*float*)
***_diffrn_reflns_transf_matrix_12*** (*cif_core.dic 2.0.1*)
The [1][2] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[1][3]** (*float*)
***_diffrn_reflns_transf_matrix_13*** (*cif_core.dic 2.0.1*)
The [1][3] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[2][1]** (*float*)
***_diffrn_reflns_transf_matrix_21*** (*cif_core.dic 2.0.1*)
The [2][1] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[2][2]** (*float*)
***_diffrn_reflns_transf_matrix_22*** (*cif_core.dic 2.0.1*)
The [2][2] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[2][3]** (*float*)
***_diffrn_reflns_transf_matrix_23*** (*cif_core.dic 2.0.1*)
The [2][3] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[3][1]** (*float*)
***_diffrn_reflns_transf_matrix_31*** (*cif_core.dic 2.0.1*)
The [3][1] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[3][2]** (*float*)
***_diffrn_reflns_transf_matrix_32*** (*cif_core.dic 2.0.1*)
The [3][2] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

**_diffrn_reflns.transf_matrix[3][3]** (*float*)
***_diffrn_reflns_transf_matrix_33*** (*cif_core.dic 2.0.1*)
The [3][3] element of the $3 \times 3$ matrix used to transform Miller indices in the DIFFRN_REFLN category into the Miller indices in the REFLN category.
**[diffrn_reflns]**

## DIFFRN_REFLNS_CLASS

Data items in the DIFFRN_REFLNS_CLASS category record details about the classes of reflections measured in the diffraction experiment.

Category key(s): **_diffrn_reflns_class.code**

*Example 1 – example corresponding to the one-dimensional incommensurately modulated structure of $K_2SeO_4$. Each reflection class is defined by the number $m = \sum |m_i|$, where the $m_i$ are the integer coefficients that, in addition to $h, k, l$, index the corresponding diffraction vector in the basis defined for the reciprocal lattice.*

```
loop_
     _diffrn_reflns_class.number
     _diffrn_reflns_class.d_res_high
     _diffrn_reflns_class.d_res_low
     _diffrn_reflns_class.av_R_eq
     _diffrn_reflns_class.code
     _diffrn_reflns_class.description
  1580 0.551 6.136 0.015 'Main' 'm=0; main reflections'
  1045 0.551 6.136 0.010 'Sat1' 'm=1; first-order satellites'
```

### _diffrn_reflns_class.av_R_eq (*float*)

***_diffrn_reflns_class_av_R_eq*** (*cif_core.dic 2.3*)

For each reflection class, the residual $[\sum \mathrm{av}|\Delta(I)| / \sum |\mathrm{av}(I)|]$ for symmetry-equivalent reflections used to calculate the average intensity $\mathrm{av}(I)$. The $\mathrm{av}|\Delta(I)|$ term is the average absolute difference between $\mathrm{av}(I)$ and the individual intensities.

The permitted range is $[0.0, \infty)$. **[diffrn_reflns_class]**

### _diffrn_reflns_class.av_sgI/I (*float*)

***_diffrn_reflns_class_av_sgI/I*** (*cif_core.dic 2.3*)

Measure $[\sum |\sigma(\mathrm{net}\ I)| / \sum |\mathrm{net}\ I|]$ for all measured intensities in a reflection class.

The permitted range is $[0.0, \infty)$.

Related item: **_diffrn_reflns_class.av_uI/I** (replaces).

**[diffrn_reflns_class]**

### _diffrn_reflns_class.av_uI/I (*float*)

***_diffrn_reflns_class_av_uI/I*** (*cif_core.dic 2.3*)

Measure $[\sum |u(\mathrm{net}\ I)| / \sum |\mathrm{net}\ I|]$ for all measured intensities in a reflection class.

The permitted range is $[0.0, \infty)$.

Related item: **_diffrn_reflns_class.av_sgI/I** (alternate).

**[diffrn_reflns_class]**

### *_diffrn_reflns_class.code (*code*)

***_diffrn_reflns_class_code*** (*cif_core.dic 2.3*)

The code identifying a certain reflection class.

Examples: '1', 'm1', 's2'. **[diffrn_reflns_class]**

### _diffrn_reflns_class.d_res_high (*float*)

***_diffrn_reflns_class_d_res_high*** (*cif_core.dic 2.3*)

The smallest value in ångströms for the interplanar spacings for the reflections in each measured reflection class. This is called the highest resolution for this reflection class.

The permitted range is $[0.0, \infty)$. **[diffrn_reflns_class]**

### _diffrn_reflns_class.d_res_low (*float*)

***_diffrn_reflns_class_d_res_low*** (*cif_core.dic 2.3*)

The largest value in ångströms of the interplanar spacings for the reflections for each measured reflection class. This is called the lowest resolution for this reflection class.

The permitted range is $[0.0, \infty)$. **[diffrn_reflns_class]**

### _diffrn_reflns_class.description (*text*)

***_diffrn_reflns_class_description*** (*cif_core.dic 2.3*)

Description of each reflection class.

Examples: 'm=1 first order satellites',
'H0L0 common projection reflections'. **[diffrn_reflns_class]**

### _diffrn_reflns_class.number (*int*)

***_diffrn_reflns_class_number*** (*cif_core.dic 2.3*)

The total number of measured intensities for each reflection class, excluding the systematic absences arising from centring translations.

The permitted range is $[0, \infty)$. **[diffrn_reflns_class]**

## DIFFRN_SCALE_GROUP

Data items in the DIFFRN_SCALE_GROUP category record details of the scaling factors applied to place all intensities in the reflection lists on a common scale. Scaling groups might, for example, correspond to each film in a multi-film data set or each crystal in a multi-crystal data set.

Category group(s): **inclusive_group**
**diffrn_group**

Category key(s): **_diffrn_scale_group.code**

*Example 1 – based on CAD-4 diffractometer data obtained for Yb(S-$C_5H_4N)_2$-$(THF)_4$.*

```
_diffrn_scale_group.code       A24
_diffrn_scale_group.I_net      1.021
```

### *_diffrn_scale_group.code (*code*)

***_diffrn_scale_group_code*** (*cif_core.dic 2.0.1*)

The value of **_diffrn_scale_group.code** must uniquely identify a record in the DIFFRN_SCALE_GROUP list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_diffrn_refln.scale_group_code***.

Examples: '1', '2', 'c1', 'c2'. **[diffrn_scale_group]**

### _diffrn_scale_group.I_net (*float*)

***_diffrn_scale_group_I_net*** (*cif_core.dic 2.0.1*)

The scale for a specific measurement group which is to be multiplied with the net intensity to place all intensities in the DIFFRN_REFLN or REFLN list on a common scale.

The permitted range is $[0.0, \infty)$. **[diffrn_scale_group]**

## DIFFRN_SOURCE

Data items in the DIFFRN_SOURCE category record details of the source of radiation used in the diffraction experiment.

Category group(s): **inclusive_group**
**diffrn_group**

Category key(s): **_diffrn_source.diffrn_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_diffrn_source.diffrn_id      's1'
_diffrn_source.source         'rotating anode'
_diffrn_source.type           'Rigaku RU-200'
_diffrn_source.power          50
_diffrn_source.current        180
_diffrn_source.size           '8mm x 0.4 mm broad-focus'
```

### _diffrn_source.current (*float*)

***_diffrn_source_current*** (*cif_core.dic 2.0.1*)

The current in milliamperes at which the radiation source was operated.

**[diffrn_source]**

**_diffrn_source.details** (*text*)
***_diffrn_source_details*** (*cif_core.dic 2.0.1*)
A description of special aspects of the radiation source used.
**[diffrn_source]**

* **_diffrn_source.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

**_diffrn_source.power** (*float*)
***_diffrn_source_power*** (*cif_core.dic 2.0.1*)
The power in kilowatts at which the radiation source was operated.
**[diffrn_source]**

**_diffrn_source.size** (*text*)
***_diffrn_source_size*** (*cif_core.dic 2.0.1*)
The dimensions of the source as viewed from the sample.
Examples: '8mm x 0.4 mm fine-focus', 'broad focus'. **[diffrn_source]**

**_diffrn_source.source** (*text*)
***_diffrn_radiation_source*** (*cifdic.c91 1.0*)
***_diffrn_source*** (*cif_core.dic 2.0*)
The general class of the radiation source.
Examples: 'sealed X-ray tube', 'nuclear reactor', 'spallation source', 'electron microscope', 'rotating-anode X-ray tube', 'synchrotron'.
**[diffrn_source]**

**_diffrn_source.take-off_angle** (*float*)
***_diffrn_source_take-off_angle*** (*cif_core.dic 2.3*)
The complement of the angle in degrees between the normal to the surface of the X-ray tube target and the primary X-ray beam for beams generated by traditional X-ray tubes.
The permitted range is [0.00, 90.0].
Example: '1.5'. **[diffrn_source]**

**_diffrn_source.target** (*code*)
***_diffrn_source_target*** (*cif_core.dic 2.0.1*)
The chemical element symbol for the X-ray target (usually the anode) used to generate X-rays. This can also be used for spallation sources.
The data value must be one of the following:

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | He | Li | Be | B | C | N | O | F | Ne | Na | Mg | Al | Si | P |
| S | Cl | Ar | K | Ca | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn |
| Ga | Ge | As | Se | Br | Kr | Rb | Sr | Y | Zr | Nb | Mo | Tc | Ru | Rh |
| Pd | Ag | Cd | In | Sn | Sb | Te | I | Xe | Cs | Ba | La | Ce | Pr | Nd |
| Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Hf | Ta | W | Re |
| Os | Ir | Pt | Au | Hg | Tl | Pb | Bi | Po | At | Rn | Fr | Ra | Ac | Th |
| Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lr | | |

**[diffrn_source]**

**_diffrn_source.type** (*text*)
***_diffrn_source_type*** (*cif_core.dic 2.0.1*)
The make, model or name of the source of radiation.
Examples: 'NSLS beamline X8C', 'Rigaku RU200'. **[diffrn_source]**

**_diffrn_source.voltage** (*float*)
***_diffrn_source_voltage*** (*cif_core.dic 2.0.1*)
The voltage in kilovolts at which the radiation source was operated.
**[diffrn_source]**

## DIFFRN_STANDARD_REFLN

Data items in the DIFFRN_STANDARD_REFLN category record details about the reflections treated as standards during the measurement of a set of diffraction intensities. Note that these are the individual standard reflections, not the results of the analysis of the standard reflections.
Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_standard_refln.diffrn_id**
**_diffrn_standard_refln.code**

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
loop_
_diffrn_standard_refln.diffrn_id
_diffrn_standard_refln.code
_diffrn_standard_refln.index_h
_diffrn_standard_refln.index_k
_diffrn_standard_refln.index_l
 s1 1  3  2  4
 s1 1  1  9  1
 s1 1  3  0 10
```

* **_diffrn_standard_refln.code** (*code*)
***_diffrn_standard_refln_code*** (*cif_core.dic 2.0.1*)
The code identifying a reflection measured as a standard reflection with the indices **_diffrn_standard_refln.index_h**, **_diffrn_standard_refln.index_k** and **_diffrn_standard_refln.index_l**. This is the same code as the **_diffrn_refln.standard_code** in the DIFFRN_REFLN list.
*The following item(s) have an equivalent role in their respective categories:*
***_diffrn_refln.standard_code***.
Examples: '1', '2', 'c1', 'c2'. **[diffrn_standard_refln]**

* **_diffrn_standard_refln.diffrn_id**
This data item is a pointer to **_diffrn.id** in the DIFFRN category.

* **_diffrn_standard_refln.index_h** (*int*)
***_diffrn_standard_refln_index_h*** (*cif_core.dic 2.0.1*)
Miller index *h* of a standard reflection used in the diffraction measurement process.
**[diffrn_standard_refln]**

* **_diffrn_standard_refln.index_k** (*int*)
***_diffrn_standard_refln_index_k*** (*cif_core.dic 2.0.1*)
Miller index *k* of a standard reflection used in the diffraction measurement process.
**[diffrn_standard_refln]**

* **_diffrn_standard_refln.index_l** (*int*)
***_diffrn_standard_refln_index_l*** (*cif_core.dic 2.0.1*)
Miller index *l* of a standard reflection used in the diffraction measurement process.
**[diffrn_standard_refln]**

## DIFFRN_STANDARDS

Data items in the DIFFRN_STANDARDS category record details about the set of standard reflections used to monitor intensity stability during the measurement of diffraction intensities. Note that these records describe properties common to the set of standard reflections, not the standard reflections themselves.

Category group(s): **inclusive_group**
**diffrn_group**
Category key(s): **_diffrn_standards.diffrn_id**

*Example 1 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276–2277].*

```
_diffrn_standards.diffrn_id        's1'
_diffrn_standards.number           3
_diffrn_standards.interval_time    120
_diffrn_standards.decay_%          0
```

### _diffrn_standards.decay_% (*float*)

***_diffrn_standards_decay_%*** (*cif_core.dic 2.0.1*)

The percentage decrease in the mean of the intensities for the set of standard reflections from the start of the measurement process to the end. This value usually affords a measure of the overall decay in crystal quality during the diffraction measurement process. Negative values are used in exceptional instances where the final intensities are greater than the initial ones.

The permitted range is $(-\infty, 100.0]$. **[diffrn_standards]**

### *_diffrn_standards.diffrn_id

This data item is a pointer to **_diffrn.id** in the DIFFRN category.

### _diffrn_standards.interval_count (*int*)

***_diffrn_standards_interval_count*** (*cif_core.dic 2.0.1*)

The number of reflection intensities between the measurement of standard reflection intensities.

The permitted range is $[0, \infty)$. **[diffrn_standards]**

### _diffrn_standards.interval_time (*float*)

***_diffrn_standards_interval_time*** (*cif_core.dic 2.0.1*)

The time in minutes between the measurement of standard reflection intensities.

The permitted range is $[0, \infty)$. **[diffrn_standards]**

### _diffrn_standards.number (*int*)

***_diffrn_standards_number*** (*cif_core.dic 2.0.1*)

The number of unique standard reflections used during the measurement of the diffraction intensities.

The permitted range is $[0, \infty)$. **[diffrn_standards]**

### _diffrn_standards.scale_sigma (*float*)

***_diffrn_standards_scale_sigma*** (*cif_core.dic 2.0.1*)

The standard uncertainty (estimated standard deviation) of the individual mean standard scales applied to the intensity data.

The permitted range is $[0.0, \infty)$. **[diffrn_standards]**

### _diffrn_standards.scale_u (*float*)

***_diffrn_standards_scale_u*** (*cif_core.dic 2.3*)

The standard uncertainty of the individual mean standard scales applied to the intensity data.

The permitted range is $[0.0, \infty)$.

Related item: **_diffrn_standards.scale_sigma** (alternate).

**[diffrn_standards]**

## ENTITY

Data items in the ENTITY category record details (such as chemical composition, name and source) about the molecular entities that are present in the crystallographic structure. Items in the various ENTITY subcategories provide a full chemical description of these molecular entities. Entities are of three types: polymer, non-polymer and water. Note that the water category includes only water; ordered solvent such as sulfate ion or acetone would be described as individual non-polymer entities. The ENTITY category is specific to macromolecular CIF applications and replaces the function of the CHEMICAL category in the CIF core. It is important to remember that the ENTITY data are not the result of the crystallographic experiment; those results are represented by the ATOM_SITE data items. ENTITY data items describe the chemistry of the molecules under investigation and can most usefully be thought of as the ideal groups to which the structure is restrained or constrained during refinement. It is also important to remember that entities do not correspond directly to the enumeration of the contents of the asymmetric unit. Entities are described only once, even in those structures that contain multiple observations of an entity. The STRUCT_ASYM data items, which reference the entity list, describe and label the contents of the asymmetric unit.

Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity.id
_entity.type
_entity.formula_weight
_entity.details
 1 polymer      10916
;  The enzymatically competent form of HIV protease is a
   dimer. This entity corresponds to one monomer of an
   active dimer.
;
 2 non-polymer 647.2  .
 3 water        18    .
```

### _entity.details (*text*)

A description of special aspects of the entity.

**[entity]**

### _entity.formula_weight (*float*)

Formula mass in daltons of the entity.

The permitted range is $[1.0, \infty)$. **[entity]**

### *_entity.id (*code*)

The value of **_entity.id** must uniquely identify a record in the ENTITY list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_site.label_entity_id***,
***_entity_keywords.entity_id***,
***_entity_link.entity_id_1***,
***_entity_link.entity_id_2***,
***_entity_name_com.entity_id***,
***_entity_name_sys.entity_id***,
***_entity_poly.entity_id***,
***_entity_poly_seq.entity_id***,
***_entity_src_gen.entity_id***,
***_entity_src_nat.entity_id***,
***_struct_asym.entity_id***,
***_struct_ref.entity_id***. **[entity]**

**_entity.src_method** (*ucode*)
The method by which the sample for the entity was produced. Entities isolated directly from natural sources (tissues, soil samples *etc.*) are expected to have further information in the ENTITY_SRC_NAT category. Entities isolated from genetically manipulated sources are expected to have further information in the ENTITY_SRC_GEN category.
The data value must be one of the following:

| | |
|---|---|
| nat | entity isolated from a natural source |
| man | entity isolated from a genetically manipulated source |
| syn | entity obtained synthetically |

**[entity]**

**_entity.type** (*ucode*)
Defines the type of the entity. Polymer entities are expected to have corresponding ENTITY_POLY and associated entries. Non-polymer entities are expected to have corresponding CHEM_COMP and associated entries. Water entities are not expected to have corresponding entries in the ENTITY category.
The data value must be one of the following:

| | |
|---|---|
| polymer | entity is a polymer |
| non-polymer | entity is not a polymer |
| water | water in the solvent model |

**[entity]**

## ENTITY_KEYWORDS

Data items in the ENTITY_KEYWORDS category specify keywords relevant to the molecular entities. Note that this list of keywords is separate from the list that is used for the STRUCT_BIOL data items and is intended to provide only the information that one would know about the molecular entity *if one did not know its structure*. Hence polypeptides are simply polypeptides, not cytokines or $\beta$-$\alpha$-barrels, and polyribonucleic acids are simply poly-RNA, not transfer-RNA.
Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_keywords.entity_id**
**_entity_keywords.text**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_keywords.entity_id
_entity_keywords.text
  1  'polypeptide'
  2  'natural product, inhibitor, reduced peptide'
```

*__entity_keywords.entity_id__
This data item is a pointer to **_entity.id** in the ENTITY category.

**_entity_keywords.text** (*text*)
Keywords describing this entity.
Examples: 'polypeptide', 'natural product', 'polysaccharide'.
**[entity_keywords]**

## ENTITY_LINK

Data items in the ENTITY_LINK category give details about the links between entities.
Category group(s): **inclusive_group**
**chem_link_group**
Category key(s): **_entity_link.link_id**

**_entity_link.details** (*text*)
A description of special aspects of a link between chemical components in the structure.
**[entity_link]**

*__entity_link.entity_id_1__
The entity ID of the first of the two entities joined by the link. This data item is a pointer to **_entity.id** in the ENTITY category.

*__entity_link.entity_id_2__
The entity ID of the second of the two entities joined by the link. This data item is a pointer to **_entity.id** in the ENTITY category.

**_entity_link.entity_seq_num_1**
For a polymer entity, the sequence number in the first of the two entities containing the link. This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

**_entity_link.entity_seq_num_2**
For a polymer entity, the sequence number in the second of the two entities containing the link. This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

*__entity_link.link_id__
This data item is a pointer to **_chem_link.id** in the CHEM_LINK category.

## ENTITY_NAME_COM

Data items in the ENTITY_NAME_COM category record the common name or names associated with the entity. In some cases, the entity name may not be the same as the name of the biological structure. For example, haemoglobin $\alpha$ chain would be the entity common name, not haemoglobin.
Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_name_com.entity_id**
**_entity_name_com.name**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_name_com.entity_id
_entity_name_com.name
 1  'HIV-1 protease monomer'
 1  'HIV-1 PR monomer'
 2  'acetyl-pepstatin'
 2  'acetyl-Ile-Val-Asp-Statine-Ala-Ile-Statine'
 3  'water'
```

*__entity_name_com.entity_id__
This data item is a pointer to **_entity.id** in the ENTITY category.

*__entity_name_com.name__ (*text*)
A common name for the entity.
Examples: 'HIV protease monomer', 'hemoglobin alpha chain', '2-fluoro-1,4-dichloro benzene', 'arbutin'. **[entity_name_com]**

## ENTITY_NAME_SYS

Data items in the ENTITY_NAME_SYS category record the systematic name or names associated with the entity and the system that was used to construct the systematic name. In some cases, the entity name may not be the same as the name of the biological structure.

Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_name_sys.entity_id**
**_entity_name_sys.name**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_name_sys.entity_id
_entity_name_sys.name
  1  'EC 3.4.23.16'
  2  'acetyl-Ile-Val-Asp-Sta-Ala-Ile-Sta'
  3  water
```

* **_entity_name_sys.entity_id**
This data item is a pointer to **_entity.id** in the ENTITY category.

* **_entity_name_sys.name** (*text*)
The systematic name for the entity.
Examples: 'hydroquinone-beta-D-pyranoside', 'EC 2.1.1.1', '2-fluoro-1,4-dichlorobenzene'. **[entity_name_sys]**

**_entity_name_sys.system** (*text*)
The system used to generate the systematic name of the entity.
Examples: 'Chemical Abstracts conventions', 'enzyme convention', 'Sigma catalog'. **[entity_name_sys]**

## ENTITY_POLY

Data items in the ENTITY_POLY category record details about the polymer, such as the type of the polymer, the number of monomers and whether it has nonstandard features.

Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_poly.entity_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_poly.entity_id
_entity_poly.type
_entity_poly.nstd_chirality
_entity_poly.nstd_linkage
_entity_poly.nstd_monomer
_entity_poly.type_details
 1  polypeptide(L)  no  no  no  .
```

* **_entity_poly.entity_id**
This data item is a pointer to **_entity.id** in the ENTITY category.

**_entity_poly.nstd_chirality** (*ucode*)
A flag to indicate whether the polymer contains at least one monomer unit with chirality different from that specified in **_entity_poly.type**.
The data value must be one of the following:

| | |
|---|---|
| no | polymer contains no monomers with different chirality |
| n | abbreviation for 'no' |
| yes | polymer contains at least one monomer with different chirality |
| y | abbreviation for 'yes' |

**[entity_poly]**

**_entity_poly.nstd_linkage** (*ucode*)
A flag to indicate whether the polymer contains at least one monomer-to-monomer link different from that implied by **_entity_poly.type**.
The data value must be one of the following:

| | |
|---|---|
| no | polymer contains no different links |
| n | abbreviation for 'no' |
| yes | polymer contains at least one different link |
| y | abbreviation for 'yes' |

**[entity_poly]**

**_entity_poly.nstd_monomer** (*ucode*)
A flag to indicate whether the polymer contains at least one monomer that is not considered standard.
The data value must be one of the following:

| | |
|---|---|
| no | polymer contains no nonstandard monomers |
| n | abbreviation for 'no' |
| yes | polymer contains at least one nonstandard monomer |
| y | abbreviation for 'yes' |

**[entity_poly]**

**_entity_poly.number_of_monomers** (*int*)
The number of monomers in the polymer.
The permitted range is $[1, \infty)$. **[entity_poly]**

**_entity_poly.type** (*ucode*)
The type of the polymer.
The data value must be one of the following:

polypeptide(D)
polypeptide(L)
polydeoxyribonucleotide
polyribonucleotide
polysaccharide(D)
polysaccharide(L)
other

**[entity_poly]**

**_entity_poly.type_details** (*text*)
A description of special aspects of the polymer type.
Examples: 'monomer Ala 16 is a D-amino acid', 'the oligomer contains alternating RNA and DNA units'.
**[entity_poly]**

## ENTITY_POLY_SEQ

Data items in the ENTITY_POLY_SEQ category specify the sequence of monomers in a polymer. Allowance is made for the possibility of microheterogeneity in a sample by allowing a given sequence number to be correlated with more than one monomer ID. The corresponding ATOM_SITE entries should reflect this heterogeneity.

Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_poly_seq.entity_id**
**_entity_poly_seq.num**
**_entity_poly_seq.mon_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_poly_seq.entity_id
_entity_poly_seq.num
_entity_poly_seq.mon_id
  1  1  PRO   1  2  GLN   1  3  ILE   1  4  THR   1  5  LEU
  1  6  TRP   1  7  GLN   1  8  ARG   1  9  PRO   1 10  LEU
  1 11  VAL   1 12  THR   1 13  ILE   1 14  LYS   1 15  ILE
  1 16  GLY   1 17  GLY   1 18  GLN   1 19  LEU   1 20  LYS
  1 21  GLU   1 22  ALA   1 23  LEU   1 24  LEU   1 25  ASP
# - - - - data truncated for brevity - - - -
```

*__entity_poly_seq.entity_id__
This data item is a pointer to __entity.id__ in the ENTITY category.

__entity_poly_seq.hetero__ (*ucode*)
A flag to indicate whether this monomer in the polymer is heterogeneous in sequence. This would be rare.
The data value must be one of the following:

| | |
|---|---|
| no | sequence is not heterogeneous at this monomer |
| n | abbreviation for 'no' |
| yes | sequence is heterogeneous at this monomer |
| y | abbreviation for 'yes' |

Where no value is given, the assumed value is 'no'. **[entity_poly_seq]**

*__entity_poly_seq.mon_id__
This data item is a pointer to __chem_comp.id__ in the CHEM_COMP category.

*__entity_poly_seq.num__ (*int*)
The value of __entity_poly_seq.num__ must uniquely and sequentially identify a record in the ENTITY_POLY_SEQ list. Note that this item must be a number and that the sequence numbers must progress in increasing numerical order.
*The following item(s) have an equivalent role in their respective categories:*
__atom_site.label_seq_id__,
__entity_link.entity_seq_num_1__,
__entity_link.entity_seq_num_2__,
__geom_angle.atom_site_label_seq_id_1__,
__geom_angle.atom_site_label_seq_id_2__,
__geom_angle.atom_site_label_seq_id_3__,
__geom_bond.atom_site_label_seq_id_1__,
__geom_bond.atom_site_label_seq_id_2__,
__geom_contact.atom_site_label_seq_id_1__,
__geom_contact.atom_site_label_seq_id_2__,
__geom_hbond.atom_site_label_seq_id_A__,
__geom_hbond.atom_site_label_seq_id_D__,
__geom_hbond.atom_site_label_seq_id_H__,
__geom_torsion.atom_site_label_seq_id_1__,
__geom_torsion.atom_site_label_seq_id_2__,
__geom_torsion.atom_site_label_seq_id_3__,
__geom_torsion.atom_site_label_seq_id_4__,
__struct_conf.beg_label_seq_id__,
__struct_conf.end_label_seq_id__,
__struct_conn.ptnr1_label_seq_id__,
__struct_conn.ptnr2_label_seq_id__,
__struct_mon_nucl.label_seq_id__,
__struct_mon_prot.label_seq_id__,
__struct_mon_prot_cis.label_seq_id__,
__struct_ncs_dom_lim.beg_label_seq_id__,
__struct_ncs_dom_lim.end_label_seq_id__,
__struct_ref_seq.seq_align_beg__,
__struct_ref_seq.seq_align_end__,
__struct_ref_seq_dif.seq_num__,
__struct_sheet_hbond.range_1_beg_label_seq_id__,
__struct_sheet_hbond.range_1_end_label_seq_id__,
__struct_sheet_hbond.range_2_beg_label_seq_id__,
__struct_sheet_hbond.range_2_end_label_seq_id__,
__struct_sheet_range.beg_label_seq_id__,
__struct_sheet_range.end_label_seq_id__,
__struct_site_gen.label_seq_id__.
The permitted range is $[1, \infty)$. **[entity_poly_seq]**

## ENTITY_SRC_GEN

Data items in the ENTITY_SRC_GEN category record details of the source from which the entity was obtained in cases where the source was genetically manipulated. The following are treated separately: items pertaining to the tissue from which the gene was obtained, items pertaining to the host organism for gene expression and items pertaining to the actual producing organism (plasmid).
Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_src_gen.entity_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_src_gen.entity_id
_entity_src_gen.gene_src_common_name
_entity_src_gen.gene_src_genus
_entity_src_gen.gene_src_species
_entity_src_gen.gene_src_strain
_entity_src_gen.host_org_common_name
_entity_src_gen.host_org_genus
_entity_src_gen.host_org_species
_entity_src_gen.plasmid_name
 1  'HIV-1'  ?  ?  'NY-5'
    'bacteria'  'Escherichia'  'coli'  'pB322'
```

*__entity_src_gen.entity_id__
This data item is a pointer to __entity.id__ in the ENTITY category.

__entity_src_gen.gene_src_common_name__ (*text*)
The common name of the natural organism from which the gene was obtained.
Examples: 'man', 'yeast', 'bacteria'. **[entity_src_gen]**

__entity_src_gen.gene_src_details__ (*text*)
A description of special aspects of the natural organism from which the gene was obtained.
**[entity_src_gen]**

__entity_src_gen.gene_src_genus__ (*text*)
The genus of the natural organism from which the gene was obtained.
Examples: 'Homo', 'Saccharomyces', 'Escherichia'. **[entity_src_gen]**

__entity_src_gen.gene_src_species__ (*text*)
The species of the natural organism from which the gene was obtained.
Examples: 'sapiens', 'cerevisiae', 'coli'. **[entity_src_gen]**

__entity_src_gen.gene_src_strain__ (*text*)
The strain of the natural organism from which the gene was obtained, if relevant.
Examples: 'DH5a', 'BMH 71-18'. **[entity_src_gen]**

__entity_src_gen.gene_src_tissue__ (*text*)
The tissue of the natural organism from which the gene was obtained.
Examples: 'heart', 'liver', 'eye lens'. **[entity_src_gen]**

__entity_src_gen.gene_src_tissue_fraction__ (*text*)
The subcellular fraction of the tissue of the natural organism from which the gene was obtained.
Examples: 'mitochondria', 'nucleus', 'membrane'. **[entity_src_gen]**

__entity_src_gen.host_org_common_name__ (*text*)
The common name of the organism that served as host for the production of the entity.
Examples: 'yeast', 'bacteria'. **[entity_src_gen]**

**_entity_src_gen.host_org_details** (*text*)
A description of special aspects of the organism that served as host for the production of the entity.

**[entity_src_gen]**

**_entity_src_gen.host_org_genus** (*text*)
The genus of the organism that served as host for the production of the entity.
Examples: 'Saccharomyces', 'Escherichia'. **[entity_src_gen]**

**_entity_src_gen.host_org_species** (*text*)
The species of the organism that served as host for the production of the entity.
Examples: 'cerevisiae', 'coli'. **[entity_src_gen]**

**_entity_src_gen.host_org_strain** (*text*)
The strain of the organism that served as host for the production of the entity.
Examples: 'DH5a', 'BMH 71-18'. **[entity_src_gen]**

**_entity_src_gen.plasmid_details** (*text*)
A description of special aspects of the plasmid that produced the entity in the host organism.

**[entity_src_gen]**

**_entity_src_gen.plasmid_name** (*text*)
The name of the plasmid that produced the entity in the host organism.
Examples: 'pET3C', 'pT123sab'. **[entity_src_gen]**

## ENTITY_SRC_NAT

Data items in the ENTITY_SRC_NAT category record details of the source from which the entity was obtained in cases where the entity was isolated directly from a natural tissue.
Category group(s): **inclusive_group**
**entity_group**
Category key(s): **_entity_src_nat.entity_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_entity_src_nat.entity_id
_entity_src_nat.common_name
_entity_src_nat.genus
_entity_src_nat.species
_entity_src_nat.details
 2  'bacteria'  'Actinomycetes' ?
;    Acetyl-pepstatin was isolated by Dr. K. Oda, Osaka
     Prefecture University, and provided to us by Dr. Ben
     Dunn, University of Florida, and Dr. J. Kay, University
     of Wales.
;
```

* **_entity_src_nat.common_name** (*text*)
The common name of the organism from which the entity was isolated.
Examples: 'man', 'yeast', 'bacteria'. **[entity_src_nat]**

**_entity_src_nat.details** (*text*)
A description of special aspects of the organism from which the entity was isolated.

**[entity_src_nat]**

* **_entity_src_nat.entity_id**
This data item is a pointer to **_entity.id** in the ENTITY category.

* **_entity_src_nat.genus** (*text*)
The genus of the organism from which the entity was isolated.
Examples: 'Homo', 'Saccharomyces', 'Escherichia'. **[entity_src_nat]**

* **_entity_src_nat.species** (*text*)
The species of the organism from which the entity was isolated.
Examples: 'sapiens', 'cerevisiae', 'coli'. **[entity_src_nat]**

* **_entity_src_nat.strain** (*text*)
The strain of the organism from which the entity was isolated.
Examples: 'DH5a', 'BMH 71-18'. **[entity_src_nat]**

* **_entity_src_nat.tissue** (*text*)
The tissue of the organism from which the entity was isolated.
Examples: 'heart', 'liver', 'eye lens'. **[entity_src_nat]**

* **_entity_src_nat.tissue_fraction** (*text*)
The subcellular fraction of the tissue of the organism from which the entity was isolated.
Examples: 'mitochondria', 'nucleus', 'membrane'. **[entity_src_nat]**

## ENTRY

There is only one item in the ENTRY category, **_entry.id**. This data item gives a name to this entry and is indirectly a key to the categories (such as CELL, GEOM, EXPTL) that describe information pertinent to the entire data block.
Category group(s): **inclusive_group**
**entry_group**
Category key(s): **_entry.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_entry.id                                   '5HVP'
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276–2277].*

```
_entry.id                                   'TOZ'
```

* **_entry.id** (*code*)
**_audit_block_code** (*cif_core.dic 2.0.1*)
The value of **_entry.id** identifies the data block. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
**_atom_sites.entry_id**,
**_cell.entry_id**,
**_cell_measurement.entry_id**,
**_chemical.entry_id**,
**_chemical_formula.entry_id**,
**_computing.entry_id**,
**_database.entry_id**,
**_database_PDB_matrix.entry_id**,
**_entry_link.entry_id**,
**_exptl.entry_id**,
**_geom.entry_id**,
**_journal.entry_id**,
**_phasing_averaging.entry_id**,
**_phasing_isomorphous.entry_id**,
**_phasing_MAD.entry_id**,
**_phasing_MIR.entry_id**,
**_publ.entry_id**,
**_publ_manuscript_incl.entry_id**,

*_refine.entry_id*,
*_refine_analyze.entry_id*,
*_reflns.entry_id*,
*_struct.entry_id*,
*_struct_keywords.entry_id*,
*_struct_mon_details.entry_id*,
*_symmetry.entry_id*. **[entry]**

## ENTRY_LINK

Data items in the ENTRY_LINK category record the relationships between the current data block identified by **_entry.id** and other data blocks within the current file which may be referenced in the current data block.

Category group(s): **inclusive_group**
**entry_group**
Category key(s): **_entry_link.id**
**_entry_link.entry_id**

*Example 1 – example file for the one-dimensional incommensurately modulated structure of $K_2SeO_4$.*

```
loop_
_entry_link.id
_entry_link.entry_id
_entry_link.details
 KSE_COM  KSE_TEXT
     'experimental data common to ref./mod. structures'
 KSE_REF  KSE_TEXT  'reference structure'
 KSE_MOD  KSE_TEXT  'modulated structure'
```

### _entry_link.details (*text*)

*_audit_link_block_description* (*cif_core.dic 2.0.1*)

A description of the relationship between the data blocks identified by **_entry_link.id** and **_entry_link.entry_id**.

**[entry_link]**

### *_entry_link.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### *_entry_link.id (*code*)

*_audit_link_block_code* (*cif_core.dic 2.0.1*)

The value of **_entry_link.id** identifies a data block related to the current data block.

**[entry_link]**

## EXPTL

Data items in the EXPTL category record details about the experimental work prior to the intensity measurements and details about the absorption-correction technique employed.

Category group(s): **inclusive_group**
**exptl_group**
Category key(s): **_exptl.entry_id**

*Example 1 – based on laboratory records for $Yb(S\text{-}C_5H_4N)_2(THF)_4$.*

```
_exptl.entry_id                    datablock1
_exptl.absorpt_coefficient_mu      1.22
_exptl.absorpt_correction_T_max    0.896
_exptl.absorpt_correction_T_min    0.802
_exptl.absorpt_correction_type     integration
_exptl.absorpt_process_details
; Gaussian grid method from SHELX76
  Sheldrick, G. M., "SHELX-76: structure determination and
  refinement program", Cambridge University, UK, 1976
;
_exptl.crystals_number             1
_exptl.details
; Enraf-Nonius LT2 liquid nitrogen variable-temperature
  device used
;
_exptl.method            'single-crystal x-ray diffraction'
_exptl.method_details
; graphite monochromatized Cu K(alpha) fixed tube and
  Enraf-Nonius CAD4 diffractometer used
;
```

### _exptl.absorpt_coefficient_mu (*float*)

*_exptl_absorpt_coefficient_mu* (*cif_core.dic 2.0.1*)

The absorption coefficient $\mu$ in reciprocal millimetres calculated from the atomic content of the cell, the density and the radiation wavelength.

The permitted range is $[0.0, \infty)$. **[exptl]**

### _exptl.absorpt_correction_T_max (*float*)

*_exptl_absorpt_correction_T_max* (*cif_core.dic 2.0.1*)

The maximum transmission factor for the crystal and radiation. The maximum and minimum transmission factors are also referred to as the absorption correction $A$ or $1/A^*$.

The permitted range is [0.0, 1.0]. **[exptl]**

### _exptl.absorpt_correction_T_min (*float*)

*_exptl_absorpt_correction_T_min* (*cif_core.dic 2.0.1*)

The minimum transmission factor for the crystal and radiation. The maximum and minimum transmission factors are also referred to as the absorption correction $A$ or $1/A^*$.

The permitted range is [0.0, 1.0]. **[exptl]**

### _exptl.absorpt_correction_type (*ucode*)

*_exptl_absorpt_correction_type* (*cif_core.dic 2.0.1*)

The absorption correction type and method. The value 'empirical' should *not* be used unless more detailed information is not available.

The data value must be one of the following:

| | |
|---|---|
| analytical | analytical from crystal shape |
| cylinder | cylindrical |
| empirical | empirical from intensities |
| gaussian | Gaussian from crystal shape |
| integration | integration from crystal shape |
| multi-scan | symmetry-related measurements |
| none | no correction applied |
| numerical | numerical from crystal shape |
| psi-scan | $\psi$-scan corrections |
| refdelf | refined from $\Delta F$ |
| sphere | spherical |

**[exptl]**

### _exptl.absorpt_process_details (*text*)

*_exptl_absorpt_process_details* (*cif_core.dic 2.0.1*)

Description of the absorption process applied to the intensities. A literature reference should be supplied for $\psi$-scan techniques.

Example: 'Tompa analytical'. **[exptl]**

### _exptl.crystals_number (*int*)

*_exptl_crystals_number* (*cif_core.dic 2.0.1*)

The total number of crystals used in the measurement of intensities.

The permitted range is $[1, \infty)$. **[exptl]**

### _exptl.details (*text*)

*_exptl_special_details* (*cif_core.dic 2.0.1*)

Any special information about the experimental work prior to the intensity measurement. See also **_exptl_crystal.preparation**.

**[exptl]**

### *_exptl.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### *_exptl.method (*line*)

The method used in the experiment.

Examples: 'single-crystal x-ray diffraction',
'single-crystal neutron diffraction',
'single-crystal electron diffraction', 'fiber x-ray diffraction',
'fiber neutron diffraction', 'fiber electron diffraction',
'single-crystal joint x-ray and neutron diffraction',
'single-crystal joint x-ray and electron diffraction',
'solution nmr', 'solid-state nmr', 'theoretical model', 'other'.

**[exptl]**

**_exptl.method_details** (*text*)

A description of special aspects of the experimental method.

Examples: '29 structures', 'minimized average structure'. **[exptl]**

## EXPTL_CRYSTAL

Data items in the EXPTL_CRYSTAL category record the results of experimental measurements on the crystal or crystals used, such as shape, size or density.

Category group(s): **inclusive_group**
**exptl_group**

Category key(s): **_exptl_crystal.id**

*Example 1 – based on laboratory records for $Yb(S\text{-}C_5H_4N)_2(THF)_4$.*

```
_exptl_crystal.id                   xst21
_exptl_crystal.colour               'pale yellow'
_exptl_crystal.density_diffrn       1.113
_exptl_crystal.density_Matthews     1.01
_exptl_crystal.density_meas         1.11
_exptl_crystal.density_meas_temp    294.5
_exptl_crystal.density_method       'neutral buoyancy'
_exptl_crystal.density_percent_sol 0.15
                                 # P = 1 - (1.23*N*MMass) / V
_exptl_crystal.description          'hexagonal rod, uncut'
_exptl_crystal.F_000                202
_exptl_crystal.preparation
; hanging drop, crystal soaked in 10% ethylene glycol for
  10 h, then placed in nylon loop at data collection time
;
_exptl_crystal.size_max             0.30
_exptl_crystal.size_mid             0.20
_exptl_crystal.size_min             0.05
_exptl_crystal.size_rad             0.025
```

*Example 2 - using separate items to define upper and lower limits for a value.*

```
_exptl_crystal.density_meas_gt      2.5
_exptl_crystal.density_meas_lt      5.0
```

*Example 3 - here the density was measured at some unspecified temperature below room temperature.*

```
_exptl_crystal.density_meas_temp_lt  300
```

**_exptl_crystal.colour** (*line*)

***_exptl_crystal_colour*** (*cif_core.dic 2.0.1*)

The colour of the crystal.

Example: 'dark green'. **[exptl_crystal]**

**_exptl_crystal.colour_lustre** (*line*)

***_exptl_crystal_colour_lustre*** (*cif_core.dic 2.3*)

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of **_exptl_crystal.colour_modifier** with **_exptl_crystal.colour_primary**, as in 'dark-green' or 'bluish-violet', if necessary combined with **_exptl_crystal.colour_lustre**, as in 'metallic-green'.

Related item: **_exptl_crystal.colour** (alternate).

The data value must be one of the following:

metallic
dull
clear **[exptl_crystal]**

**_exptl_crystal.colour_modifier** (*line*)

***_exptl_crystal_colour_modifier*** (*cif_core.dic 2.3*)

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of **_exptl_crystal.colour_modifier** with **_exptl_crystal.colour_primary**, as in 'dark-green' or 'bluish-violet', if necessary combined with **_exptl_crystal.colour_lustre**, as in 'metallic-green'.

Related item: **_exptl_crystal.colour** (alternate).

The data value must be one of the following:

light
dark
whitish
blackish
grayish
brownish
reddish
pinkish
orangish
yellowish
greenish
bluish **[exptl_crystal]**

**_exptl_crystal.colour_primary** (*line*)

***_exptl_crystal_colour_primary*** (*cif_core.dic 2.3*)

The enumeration list of standardized names developed for the International Centre for Diffraction Data. The colour of a crystal is given by the combination of **_exptl_crystal.colour_modifier** with **_exptl_crystal.colour_primary**, as in 'dark-green' or 'bluish-violet', if necessary combined with **_exptl_crystal.colour_lustre**, as in 'metallic-green'.

Related item: **_exptl_crystal.colour** (alternate).

The data value must be one of the following:

colourless
white
black
gray
brown
red
pink
orange
yellow
green
blue
violet **[exptl_crystal]**

**_exptl_crystal.density_diffrn** (*float*)

***_exptl_crystal_density_diffrn*** (*cif_core.dic 2.0.1*)

Density values calculated from the crystal cell and contents. The units are megagrams per cubic metre (grams per cubic centimetre).

The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.density_Matthews** (*float*)

The density of the crystal, expressed as the ratio of the volume of the asymmetric unit to the molecular mass of a monomer of the structure, in units of ångströms$^3$ per dalton.

Reference: Matthews, B. W. (1968). *J. Mol. Biol.* **33**, 491–497.

**[exptl_crystal]**

**_exptl_crystal.density_meas** (*float, su*)

***_exptl_crystal_density_meas*** (*cif_core.dic 2.3*)

Density values measured using standard chemical and physical methods. The units are megagrams per cubic metre (grams per cubic centimetre).

The permitted range is $[0.0, \infty)$.

Related item: **_exptl_crystal.density_meas_esd** (associated esd).

**[exptl_crystal]**

**_exptl_crystal.density_meas_esd** (*float*)

The standard uncertainty (estimated standard deviation) of **_exptl_crystal.density_meas**.

Related item: **_exptl_crystal.density_meas** (associated value).

**[exptl_crystal]**

**_exptl_crystal.density_meas_gt** (*float*)
***_exptl_crystal_density_meas_gt*** (*cif_core.dic 2.3*)
The value above which the density measured using standard chemical and physical methods lies. The units are megagrams per cubic metre (grams per cubic centimetre). **_exptl_crystal.density_meas_gt** and **_exptl_crystal.density_meas_lt** should not be used to report new experimental work, for which **_exptl_crystal.density_meas** should be used. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under **_exptl_crystal.density_meas**.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal.density_meas** (alternate) .
Example: '2.5' (lower limit for the density (only the range within which the density lies was given in the original paper)). **[exptl_crystal]**

**_exptl_crystal.density_meas_lt** (*float*)
***_exptl_crystal_density_meas_lt*** (*cif_core.dic 2.3*)
The value below which the density measured using standard chemical and physical methods lies. The units are megagrams per cubic metre (grams per cubic centimetre). **_exptl_crystal.density_meas_gt** and **_exptl_crystal.density_meas_lt** should not be used to report new experimental work, for which **_exptl_crystal.density_meas** should be used. These items are intended for use in reporting information in existing databases and archives which would be misleading if reported under **_exptl_crystal.density_meas**.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal.density_meas** (alternate) .
Examples: '1.0' (specimen floats in water), '5.0' (upper limit for the density (only the range within which the density lies was given in the original paper)). **[exptl_crystal]**

**_exptl_crystal.density_meas_temp** (*float, su*)
***_exptl_crystal_density_meas_temp*** (*cif_core.dic 2.3*)
Temperature in kelvins at which **_exptl_crystal.density_meas** was determined.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.density_meas_temp_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_exptl_crystal.density_meas_temp**.
**[exptl_crystal]**

**_exptl_crystal.density_meas_temp_gt** (*float*)
***_exptl_crystal_density_meas_temp_gt*** (*cif_core.dic 2.3*)
Temperature in kelvins above which **_exptl_crystal.density_meas** was determined. **_exptl_crystal.density_meas_temp_gt** and **_exptl_crystal.density_meas_temp_lt** should not be used for reporting new work, for which the correct temperature of measurement should be given. These items are intended for use in reporting information stored in databases or archives which would be misleading if reported under **_exptl_crystal.density_meas_temp**.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal.density_meas_temp** (alternate).
**[exptl_crystal]**

**_exptl_crystal.density_meas_temp_lt** (*float*)
***_exptl_crystal_density_meas_temp_lt*** (*cif_core.dic 2.3*)
Temperature in kelvins below which **_exptl_crystal.density_meas** was determined. **_exptl_crystal.density_meas_temp_gt** and **_exptl_crystal.density_meas_temp_lt** should not be used for reporting new work, for which the correct temperature of measurement should be given. These items are intended for use in reporting information stored in databases or archives which would be misleading if reported under **_exptl_crystal.density_meas_temp**.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal.density_meas_temp** (alternate) .
Example: '300' (The density was measured at some unspecified temperature below room temperature.). **[exptl_crystal]**

**_exptl_crystal.density_method** (*text*)
***_exptl_crystal_density_method*** (*cif_core.dic 2.0.1*)
The method used to measure **_exptl_crystal.density_meas**.
**[exptl_crystal]**

**_exptl_crystal.density_percent_sol** (*float*)
Density value $P$ calculated from the crystal cell and contents, expressed as per cent solvent.

$$P = 1 - (1.23 N M_{\mathrm{Mass}})/V,$$

where $N$ = the number of molecules in the unit cell, $M_{\mathrm{Mass}}$ = the molecular mass of each molecule (g mol$^{-1}$), $V$ = the volume of the unit cell (Å$^3$) and 1.23 = a conversion factor evaluated as

$$\frac{(0.74\mathrm{cm}^3/\mathrm{g})(10^{24}\text{Å}^3/\mathrm{cm}^3)}{(6.02 \times 10^{23}\mathrm{molecules/mole})},$$

where 0.74 is an assumed value for the partial specific volume of the molecule.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.description** (*text*)
***_exptl_crystal_description*** (*cif_core.dic 2.0.1*)
A description of the quality and habit of the crystal. The crystal dimensions should not normally be reported here; use instead the specific items in the EXPTL_CRYSTAL category relating to size for the gross dimensions of the crystal and data items in the EXPTL_CRYSTAL_FACE category to describe the relationship between individual faces.
**[exptl_crystal]**

**_exptl_crystal.F_000** (*int*)
***_exptl_crystal_F_000*** (*cif_core.dic 2.0.1*)
The effective number of electrons in the crystal unit cell contributing to $F(000)$. This may contain dispersion contributions and is calculated as

$$F(000) = \left[\left(\sum f_r\right)^2 + \left(\sum f_i\right)^2\right]^{1/2},$$

where $f_r$ = real part of the scattering factors at $\theta = 0°$, $f_i$ = imaginary part of the scattering factors at $\theta = 0°$ and the sum is taken over each atom in the unit cell.
The permitted range is $[1, \infty)$. **[exptl_crystal]**

***_exptl_crystal.id** (*code*)
***_exptl_crystal_id*** (*cif_core.dic 2.0.1*)
The value of **_exptl_crystal.id** must uniquely identify a record in the EXPTL_CRYSTAL list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_diffrn.crystal_id***,
***_exptl_crystal_grow.crystal_id***,
***_exptl_crystal_face.crystal_id***,
***_exptl_crystal_grow_comp.crystal_id***,
***_refln.crystal_id***. **[exptl_crystal]**

**_exptl_crystal.preparation** (*text*)
***_exptl_crystal_preparation*** (*cif_core.dic 2.0.1*)
Details of crystal growth and preparation of the crystal (*e.g.* mounting) prior to the intensity measurements.
Example: 'mounted in an argon-filled quartz capillary'.
**[exptl_crystal]**

**_exptl_crystal.size_max** (*float*)
***_exptl_crystal_size_max*** (*cif_core.dic 2.0.1*)
The maximum dimension of the crystal. This item may appear in a list with **_exptl_crystal.id** if multiple crystals are used in the experiment.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.size_mid** (*float*)
***_exptl_crystal_size_mid*** (*cif_core.dic 2.0.1*)
The medial dimension of the crystal. This item may appear in a list with **_exptl_crystal.id** if multiple crystals are used in the experiment.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.size_min** (*float*)
***_exptl_crystal_size_min*** (*cif_core.dic 2.0.1*)
The minimum dimension of the crystal. This item may appear in a list with **_exptl_crystal.id** if multiple crystals are used in the experiment.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

**_exptl_crystal.size_rad** (*float*)
***_exptl_crystal_size_rad*** (*cif_core.dic 2.0.1*)
The radius of the crystal, if the crystal is a sphere or a cylinder. This item may appear in a list with **_exptl_crystal.id** if multiple crystals are used in the experiment.
The permitted range is $[0.0, \infty)$. **[exptl_crystal]**

## EXPTL_CRYSTAL_FACE

Data items in the EXPTL_CRYSTAL_FACE category record details of the crystal faces.
Category group(s): **inclusive_group**
**exptl_group**
Category key(s): **_exptl_crystal_face.crystal_id**
**_exptl_crystal_face.index_h**
**_exptl_crystal_face.index_k**
**_exptl_crystal_face.index_l**

*Example 1 – based on laboratory records for $Yb(S\text{-}C_5H_4N)_2(THF)_4$ for the 100 face of crystal xstl1.*

```
_exptl_crystal_face.crystal_id    xstl1
_exptl_crystal_face.index_h       1
_exptl_crystal_face.index_k       0
_exptl_crystal_face.index_l       0
_exptl_crystal_face.diffr_chi     42.56
_exptl_crystal_face.diffr_kappa   30.23
_exptl_crystal_face.diffr_phi     -125.56
_exptl_crystal_face.diffr_psi     -0.34
_exptl_crystal_face.perp_dist     0.025
```

***_exptl_crystal_face.crystal_id**
This data item is a pointer to **_exptl_crystal.id** in the EXPTL_CRYSTAL category.

**_exptl_crystal_face.diffr_chi** (*float*)
***_exptl_crystal_face_diffr_chi*** (*cif_core.dic 2.0.1*)
The $\chi$ diffractometer setting angle in degrees for a specific crystal face associated with **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

**_exptl_crystal_face.diffr_kappa** (*float*)
***_exptl_crystal_face_diffr_kappa*** (*cif_core.dic 2.0.1*)
The $\kappa$ diffractometer setting angle in degrees for a specific crystal face associated with **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

**_exptl_crystal_face.diffr_phi** (*float*)
***_exptl_crystal_face_diffr_phi*** (*cif_core.dic 2.0.1*)
The $\varphi$ diffractometer setting angle in degrees for a specific crystal face associated with **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

**_exptl_crystal_face.diffr_psi** (*float*)
***_exptl_crystal_face_diffr_psi*** (*cif_core.dic 2.0.1*)
The $\psi$ diffractometer setting angle in degrees for a specific crystal face associated with **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

***_exptl_crystal_face.index_h** (*int*)
***_exptl_crystal_face_index_h*** (*cif_core.dic 2.0.1*)
Miller index $h$ of the crystal face associated with the value **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

***_exptl_crystal_face.index_k** (*int*)
***_exptl_crystal_face_index_k*** (*cif_core.dic 2.0.1*)
Miller index $k$ of the crystal face associated with the value **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

***_exptl_crystal_face.index_l** (*int*)
***_exptl_crystal_face_index_l*** (*cif_core.dic 2.0.1*)
Miller index $l$ of the crystal face associated with the value **_exptl_crystal_face.perp_dist**.
**[exptl_crystal_face]**

**_exptl_crystal_face.perp_dist** (*float*)
***_exptl_crystal_face_perp_dist*** (*cif_core.dic 2.0.1*)
The perpendicular distance in millimetres from the face to the centre of rotation of the crystal.
The permitted range is $[0.0, \infty)$. **[exptl_crystal_face]**

## EXPTL_CRYSTAL_GROW

Data items in the EXPTL_CRYSTAL_GROW category record details about the conditions and methods used to grow the crystal.
Category group(s): **inclusive_group**
**exptl_group**
Category key(s): **_exptl_crystal_grow.crystal_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_exptl_crystal_grow.crystal_id     1
_exptl_crystal_grow.method         'hanging drop'
_exptl_crystal_grow.apparatus      'Linbro plates'
_exptl_crystal_grow.atmosphere     'room air'
_exptl_crystal_grow.pH             4.7
_exptl_crystal_grow.temp           18(3)
_exptl_crystal_grow.time           'approximately 2 days'
```

**_exptl_crystal_grow.apparatus** (*text*)
The physical apparatus in which the crystal was grown.
Examples: 'Linbro plate', 'sandwich box', 'ACA plates'.
**[exptl_crystal_grow]**

**_exptl_crystal_grow.atmosphere** (*text*)
The nature of the gas or gas mixture in which the crystal was grown.
Examples: 'room air', 'nitrogen', 'argon'. **[exptl_crystal_grow]**

*_exptl_crystal_grow.crystal_id
This data item is a pointer to **_exptl_crystal.id** in the EXPTL_CRYSTAL category.

**_exptl_crystal_grow.details** (*text*)
A description of special aspects of the crystal growth.
Examples:
```
; Solution 2 was prepared as a well solution and
  mixed. A droplet containing 2 \ml of solution
  1 was delivered onto a cover slip; 2 \ml of
  solution 2 was added to the droplet without
  mixing.
;
; Crystal plates were originally stored at room
  temperature for 1 week but no nucleation
  occurred. They were then transferred to 4
  degrees C, at which temperature well formed
  single crystals grew in 2 days.
;
; The dependence on pH for successful crystal
  growth is very sharp. At pH 7.4 only showers
  of tiny crystals grew, at pH 7.5 well formed
  single crystals grew, at pH 7.6 no
  crystallization occurred at all.
;
```
**[exptl_crystal_grow]**

**_exptl_crystal_grow.method** (*text*)
The method used to grow the crystals.
Examples: 'batch precipitation', 'batch dialysis', 'hanging drop vapor diffusion', 'sitting drop vapor diffusion'.
**[exptl_crystal_grow]**

**_exptl_crystal_grow.method_ref** (*text*)
A literature reference that describes the method used to grow the crystals.
Example: 'McPherson et al., 1988'. **[exptl_crystal_grow]**

**_exptl_crystal_grow.pH** (*float*)
The pH at which the crystal was grown. If more than one pH was employed during the crystallization process, the final pH should be noted here and the protocol involving multiple pH values should be described in **_exptl_crystal_grow.details**.
The permitted range is $[0.0, \infty)$.
Examples: '7.4', '7.6', '4.3'. **[exptl_crystal_grow]**

**_exptl_crystal_grow.pressure** (*float, su*)
The ambient pressure in kilopascals at which the crystal was grown.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal_grow.pressure_esd** (associated esd).
**[exptl_crystal_grow]**

**_exptl_crystal_grow.pressure_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_exptl_crystal_grow.pressure**.
Related item: **_exptl_crystal_grow.pressure** (associated value).
**[exptl_crystal_grow]**

**_exptl_crystal_grow.seeding** (*text*)
A description of the protocol used for seeding the crystal growth.
Examples: 'macroseeding',
```
; Microcrystals were introduced from a previous
  crystal growth experiment by transfer with a
  human hair.
;
```
**[exptl_crystal_grow]**

**_exptl_crystal_grow.seeding_ref** (*text*)
A literature reference that describes the protocol used to seed the crystal.
Example: 'Stura et al., 1989'. **[exptl_crystal_grow]**

**_exptl_crystal_grow.temp** (*float, su*)
The temperature in kelvins at which the crystal was grown. If more than one temperature was employed during the crystallization process, the final temperature should be noted here and the protocol involving multiple temperatures should be described in **_exptl_crystal_grow.details**.
The permitted range is $[0.0, \infty)$.
Related item: **_exptl_crystal_grow.temp_esd** (associated esd).
**[exptl_crystal_grow]**

**_exptl_crystal_grow.temp_details** (*text*)
A description of special aspects of temperature control during crystal growth.
**[exptl_crystal_grow]**

**_exptl_crystal_grow.temp_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_exptl_crystal_grow.temp**.
Related item: **_exptl_crystal_grow.temp** (associated value).
**[exptl_crystal_grow]**

**_exptl_crystal_grow.time** (*text*)
The approximate time that the crystal took to grow to the size used for data collection.
Examples: 'overnight', '2-4 days', '6 months'. **[exptl_crystal_grow]**

## EXPTL_CRYSTAL_GROW_COMP

Data items in the EXPTL_CRYSTAL_GROW_COMP category record details about the components of the solutions that were 'mixed' (by whatever means) to produce the crystal. In general, solution 1 is the solution that contains the molecule to be crystallized and solution 2 is the solution that contains the precipitant. However, the number of solutions required to describe the crystallization protocol is not limited to 2. Details of the crystallization protocol should be given in **_exptl_crystal_grow_comp.details** using the solutions described in EXPTL_CRYSTAL_GROW_COMP.
Category group(s): **inclusive_group**
**exptl_group**
Category key(s): **_exptl_crystal_grow_comp.id**
**_exptl_crystal_grow_comp.crystal_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_exptl_crystal_grow_comp.crystal_id
_exptl_crystal_grow_comp.id
_exptl_crystal_grow_comp.sol_id
_exptl_crystal_grow_comp.name
_exptl_crystal_grow_comp.volume
_exptl_crystal_grow_comp.conc
_exptl_crystal_grow_comp.details
 1 1  1  'HIV-1 protease'  '0.002 ml'  '6 mg/ml'
; The protein solution was in a buffer containing 25 mM NaCl,
  100 mM NaMES/ MES buffer, pH 7.5, 3 mM NaAzide
;
 1 2 2 'NaCl'         '0.200 ml'  '4    M' 'in 3 mM NaAzide'
 1 3 2 'Acetic Acid'  '0.047 ml'  '100 mM' 'in 3 mM NaAzide'
 1 4 2 'Na Acetate'   '0.053 ml'  '100 mM'
; in 3 mM NaAzide. Buffer components were mixed to produce a
  pH of 4.7 according to a ratio calculated from the pKa. The
  actual pH of solution 2 was not measured.
;
 1 5 2 'water'        '0.700 ml'   'neat'  'in 3 mM NaAzide'
```

**_exptl_crystal_grow_comp.conc** (*line*)
The concentration of the solution component.
Examples: '200 \ml', '0.1 ml'. **[exptl_crystal_grow_comp]**

*_exptl_crystal_grow_comp.crystal_id
This data item is a pointer to **_exptl_crystal.id** in the EXPTL_CRYSTAL category.

**_exptl_crystal_grow_comp.details** (*text*)
A description of any special aspects of the solution component. When the solution component is the one that contains the macromolecule, this could be the specification of the buffer in which the macromolecule was stored. When the solution component is a buffer component, this could be the methods (or formula) used to achieve a desired pH.
Examples: 'in 3 mM NaAzide',

```
; The protein solution was in a buffer
  containing 25 mM NaCl, 100 mM NaMES/MES
  buffer, pH 7.5, 3 mM NaAzide
;
; in 3 mM NaAzide. Buffer components were mixed
  to produce a pH of 4.7 according to a ratio
  calculated from the pKa. The actual pH of
  solution 2 was not measured.
;
```
**[exptl_crystal_grow_comp]**

*_exptl_crystal_grow_comp.id (*line*)
The value of **_exptl_crystal_grow_comp.id** must uniquely identify each item in the EXPTL_CRYSTAL_GROW_COMP list. Note that this item need not be a number; it can be any unique identifier.
Examples: '1', 'A', 'protein in buffer'. **[exptl_crystal_grow_comp]**

**_exptl_crystal_grow_comp.name** (*line*)
A common name for the component of the solution.
Examples: 'protein in buffer', 'acetic acid'.
**[exptl_crystal_grow_comp]**

**_exptl_crystal_grow_comp.sol_id** (*line*)
An identifier for the solution to which the given solution component belongs.
Examples: '1', 'well solution', 'solution A'. **[exptl_crystal_grow_comp]**

**_exptl_crystal_grow_comp.volume** (*line*)
The volume of the solution component.
Examples: '200 \ml', '0.1 ml'. **[exptl_crystal_grow_comp]**

## GEOM

Data items in the GEOM and related (GEOM_ANGLE, GEOM_BOND, GEOM_CONTACT, GEOM_HBOND and GEOM_TORSION) categories record details about the molecular geometry as calculated from the contents of the ATOM, CELL and SYMMETRY data. Geometry data are therefore redundant, in that they can be calculated from other more fundamental quantities in the data block. However, they provide a check on the correctness of both sets of data and enable the most important geometric data to be identified for publication by setting the appropriate publication flag.
Category group(s): **inclusive_group**
**geom_group**
Category key(s): **_geom.entry_id**

**_geom.details** (*text*)
***_geom_special_details*** (*cif_core.dic 2.0.1*)
A description of geometry not covered by the existing data names in the GEOM categories, such as least-squares planes.
**[geom]**

*_geom.entry_id
This data item is a pointer to **_entry.id** in the ENTRY category.

## GEOM_ANGLE

Data items in the GEOM_ANGLE category record details about the bond angles as calculated from the contents of the ATOM, CELL and SYMMETRY data.
Category group(s): **inclusive_group**
**geom_group**
Category key(s): **_geom_angle.atom_site_id_1**
**_geom_angle.atom_site_id_2**
**_geom_angle.atom_site_id_3**
**_geom_angle.site_symmetry_1**
**_geom_angle.site_symmetry_2**
**_geom_angle.site_symmetry_3**

*Example 1 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
loop_
_geom_angle.atom_site_id_1
_geom_angle.atom_site_id_2
_geom_angle.atom_site_id_3
_geom_angle.value
_geom_angle.value_esd
_geom_angle.site_symmetry_1
_geom_angle.site_symmetry_2
_geom_angle.site_symmetry_3
_geom_angle.publ_flag
 C2  O1  C5   111.6  0.2  1_555  1_555  1_555  yes
 O1  C2  C3   110.9  0.2  1_555  1_555  1_555  yes
 O1  C2  O21  122.2  0.3  1_555  1_555  1_555  yes
 C3  C2  O21  127.0  0.3  1_555  1_555  1_555  yes
 C2  C3  N4   101.3  0.2  1_555  1_555  1_555  yes
 C2  C3  C31  111.3  0.2  1_555  1_555  1_555  yes
 C2  C3  H3   107    1    1_555  1_555  1_555  no
 N4  C3  C31  116.7  0.2  1_555  1_555  1_555  yes
# - - - - data truncated for brevity - - - -
```

**_geom_angle.atom_site_auth_asym_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_asym_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_asym_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_atom_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_atom_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_atom_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_comp_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_comp_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_comp_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_seq_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_seq_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_angle.atom_site_auth_seq_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_geom_angle.atom_site_id_1**
***_geom_angle_atom_site_label_1*** (*cif_core.dic 2.0.1*)
The identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_angle.atom_site_id_2**
***_geom_angle_atom_site_label_2*** (*cif_core.dic 2.0.1*)
The identifier of the second of the three atom sites that define the angle. The second atom is taken to be the apex of the angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_angle.atom_site_id_3**
***_geom_angle_atom_site_label_3*** (*cif_core.dic 2.0.1*)
The identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_alt_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_alt_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_alt_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_asym_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_asym_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_asym_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_atom_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_atom_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_atom_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_comp_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_comp_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_comp_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_seq_id_1**
An optional identifier of the first of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_seq_id_2**
An optional identifier of the second of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_angle.atom_site_label_seq_id_3**
An optional identifier of the third of the three atom sites that define the angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_angle.publ_flag** (*ucode*)
***_geom_angle_publ_flag*** (*cif_core.dic 2.0.1*)
This code signals whether the angle is referred to in a publication or should be placed in a table of significant angles.
The data value must be one of the following:

| | |
|---|---|
| no | do not include angle in special list |
| n | abbreviation for 'no' |
| yes | do include angle in special list |
| y | abbreviation for 'yes' |

**[geom_angle]**

***_geom_angle.site_symmetry_1** (*symop*)
***_geom_angle_site_symmetry_1*** (*cif_core.dic 2.0.1*)
The symmetry code of the first of the three atom sites that define the angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_angle]**

***_geom_angle.site_symmetry_2** (*symop*)
***_geom_angle_site_symmetry_2*** (*cif_core.dic 2.0.1*)
The symmetry code of the second of the three atom sites that define the angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_angle]**

***_geom_angle.site_symmetry_3** (*symop*)
***_geom_angle_site_symmetry_3*** (*cif_core.dic 2.0.1*)
The symmetry code of the third of the three atom sites that define the angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_angle]**

**_geom_angle.value** (*float, su*)
***_geom_angle*** (*cif_core.dic 2.0.1*)
Angle in degrees defined by the three sites **_geom_angle.atom_site_id_1**, **_geom_angle.atom_site_id_2** and **_geom_angle.atom_site_id_3**.
Related item: **_geom_angle.value_esd** (associated esd). **[geom_angle]**

**_geom_angle.value_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_geom_angle.value**.
Related item: **_geom_angle.value** (associated value). **[geom_angle]**

## GEOM_BOND

Data items in the GEOM_BOND category record details about the bond lengths as calculated from the contents of the ATOM, CELL and SYMMETRY data.
Category group(s): **inclusive_group**
**geom_group**
Category key(s): **_geom_bond.atom_site_id_1**
**_geom_bond.atom_site_id_2**
**_geom_bond.site_symmetry_1**
**_geom_bond.site_symmetry_2**

*Example 1 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), **C47**, 2276–2277].*

```
loop_
_geom_bond.atom_site_id_1
_geom_bond.atom_site_id_2
_geom_bond.dist
_geom_bond.dist_esd
_geom_bond.site_symmetry_1
_geom_bond.site_symmetry_2
_geom_bond.publ_flag
  O1  C2   1.342 0.004  1_555  1_555  yes
  O1  C5   1.439 0.003  1_555  1_555  yes
  C2  C3   1.512 0.004  1_555  1_555  yes
  C2  O21  1.199 0.004  1_555  1_555  yes
  C3  N4   1.465 0.003  1_555  1_555  yes
  C3  C31  1.537 0.004  1_555  1_555  yes
  C3  H3   1.00  0.03   1_555  1_555  no
  N4  C5   1.472 0.003  1_555  1_555  yes
# - - - - data truncated for brevity - - - -
```

**_geom_bond.atom_site_auth_asym_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_asym_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_atom_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_atom_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_comp_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_comp_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_seq_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_bond.atom_site_auth_seq_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_geom_bond.atom_site_id_1**
***_geom_bond_atom_site_label_1*** (*cif_core.dic 2.0.1*)
The identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_bond.atom_site_id_2**
***_geom_bond_atom_site_label_2*** (*cif_core.dic 2.0.1*)
The identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_alt_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_alt_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_asym_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_asym_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_atom_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_atom_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_comp_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_comp_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_seq_id_1**
An optional identifier of the first of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_bond.atom_site_label_seq_id_2**
An optional identifier of the second of the two atom sites that define the bond. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_bond.dist** (*float, su*)
***_geom_bond_distance*** (*cif_core.dic 2.0.1*)
The intramolecular bond distance in ångströms.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_bond.dist_esd** (associated esd). **[geom_bond]**

**_geom_bond.dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_geom_bond.dist**.
Related item: **_geom_bond.dist** (associated value). **[geom_bond]**

**_geom_bond.publ_flag** (*ucode*)
***_geom_bond_publ_flag*** (*cif_core.dic 2.0.1*)
This code signals whether the bond distance is referred to in a publication or should be placed in a list of significant bond distances.
The data value must be one of the following:

| | |
|---|---|
| no | do not include bond in special list |
| n | abbreviation for 'no' |
| yes | do include bond in special list |
| y | abbreviation for 'yes' |

**[geom_bond]**

* **_geom_bond.site_symmetry_1** (*symop*)
***_geom_bond_site_symmetry_1*** (*cif_core.dic 2.0.1*)
The symmetry code of the first of the two atom sites that define the bond.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_bond]**

* **_geom_bond.site_symmetry_2** (*symop*)
***_geom_bond_site_symmetry_2*** (*cif_core.dic 2.0.1*)
The symmetry code of the second of the two atom sites that define the bond.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_bond]**

**_geom_bond.valence** (*int*)
***_geom_bond_valence*** (*cif_core.dic 2.3*)
The bond valence calculated from **_geom_bond.dist**.
**[geom_bond]**

## GEOM_CONTACT

Data items in the GEOM_CONTACT category record details about interatomic contacts as calculated from the contents of the ATOM, CELL and SYMMETRY data.

Category group(s): **inclusive_group**
**geom_group**

Category key(s): **_geom_contact.atom_site_id_1**
**_geom_contact.atom_site_id_2**
**_geom_contact.site_symmetry_1**
**_geom_contact.site_symmetry_2**

*Example 1 – based on data set CLPHO6 of Ferguson, Ruhl, McKervey & Browne [Acta Cryst. (1992), C**48**, 2262–2264].*

```
loop_
_geom_contact.atom_site_id_1
_geom_contact.atom_site_id_2
_geom_contact.dist
_geom_contact.dist_esd
_geom_contact.site_symmetry_1
_geom_contact.site_symmetry_2
_geom_contact.publ_flag
 O(1)  O(2)   2.735 0.003 .  .  yes
 H(O1) O(2)   1.82  .     .  .  no
```

**_geom_contact.atom_site_auth_asym_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_asym_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_atom_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_atom_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_comp_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_comp_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_seq_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_contact.atom_site_auth_seq_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_geom_contact.atom_site_id_1**
***_geom_contact_atom_site_label_1*** (*cif_core.dic 2.0.1*)
The identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_contact.atom_site_id_2**
***_geom_contact_atom_site_label_2*** (*cif_core.dic 2.0.1*)
The identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_alt_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_alt_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_asym_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_asym_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_atom_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_atom_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_comp_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_comp_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_seq_id_1**
An optional identifier of the first of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_contact.atom_site_label_seq_id_2**
An optional identifier of the second of the two atom sites that define the contact. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_contact.dist** (*float, su*)
***_geom_contact_distance*** (*cif_core.dic 2.0.1*)
The interatomic contact distance in ångströms.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_contact.dist_esd** (associated esd). **[geom_contact]**

**_geom_contact.dist_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_geom_contact.dist**.
Related item: **_geom_contact.dist** (associated value). **[geom_contact]**

**_geom_contact.publ_flag** (*ucode*)
***_geom_contact_publ_flag*** (*cif_core.dic 2.0.1*)
This code signals whether the contact distance is referred to in a publication or should be placed in a list of significant contact distances.
The data value must be one of the following:

| | |
|---|---|
| no | do not include distance in special list |
| n | abbreviation for 'no' |
| yes | do include distance in special list |
| y | abbreviation for 'yes' |

**[geom_contact]**

***_geom_contact.site_symmetry_1** (*symop*)
***_geom_contact_site_symmetry_1*** (*cif_core.dic 2.0.1*)
The symmetry code of the first of the two atom sites that define the contact.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_contact]**

***_geom_contact.site_symmetry_2** (*symop*)
***_geom_contact_site_symmetry_2*** (*cif_core.dic 2.0.1*)
The symmetry code of the second of the two atom sites that define the contact.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_contact]**

## GEOM_HBOND

Data items in the GEOM_HBOND category record details about hydrogen bonds as calculated from the contents of the ATOM, CELL and SYMMETRY data.
Category group(s): **inclusive_group**
**geom_group**
Category key(s): **_geom_hbond.atom_site_id_A**
**_geom_hbond.atom_site_id_D**
**_geom_hbond.atom_site_id_H**
**_geom_hbond.site_symmetry_A**
**_geom_hbond.site_symmetry_D**
**_geom_hbond.site_symmetry_H**

*Example 1 – based on $C_{14}H_{13}ClN_2O.H_2O$, reported by Palmer, Puddle & Lisgarten [Acta Cryst. (1993), C**49**, 1777–1779].*

```
loop_
_geom_hbond.atom_site_id_D
_geom_hbond.atom_site_id_H
_geom_hbond.atom_site_id_A
_geom_hbond.dist_DH
_geom_hbond.dist_HA
_geom_hbond.dist_DA
_geom_hbond.angle_DHA
_geom_hbond.publ_flag
N6   HN6  OW   0.888  1.921  2.801  169.6  yes
OW   HO2  O7   0.917  1.923  2.793  153.5  yes
OW   HO1  N10  0.894  1.886  2.842  179.7  yes
```

**_geom_hbond.angle_DHA** (*float, su*)
***_geom_hbond_angle_DHA*** (*cif_core.dic 2.0.1*)
The angle in degrees defined by the donor-, hydrogen- and acceptor-atom sites in a hydrogen bond.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_hbond.angle_DHA_esd** (associated esd). **[geom_hbond]**

**_geom_hbond.angle_DHA_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_geom_hbond.angle_DHA**.
Related item: **_geom_hbond.angle_DHA** (associated value). **[geom_hbond]**

**_geom_hbond.atom_site_auth_asym_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_asym_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_asym_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_atom_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_atom_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_atom_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_comp_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_comp_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_comp_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_seq_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_seq_id in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_seq_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_seq_id in the ATOM_SITE category.

**_geom_hbond.atom_site_auth_seq_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.auth_seq_id in the ATOM_SITE category.

* **_geom_hbond.atom_site_id_A**
*_geom_hbond_atom_site_label_A* (*cif_core.dic 2.0.1*)
The identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.id in the ATOM_SITE category.

* **_geom_hbond.atom_site_id_D**
*_geom_hbond_atom_site_label_D* (*cif_core.dic 2.0.1*)
The identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.id in the ATOM_SITE category.

* **_geom_hbond.atom_site_id_H**
*_geom_hbond_atom_site_label_H* (*cif_core.dic 2.0.1*)
The identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_alt_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_alt_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_alt_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_alt_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_alt_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_alt_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_asym_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_asym_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_asym_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_asym_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_asym_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_asym_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_atom_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_atom_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_atom_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_atom_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_atom_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_atom_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_comp_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_comp_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_comp_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_comp_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_seq_id_A**
An optional identifier of the acceptor-atom site that defines the hydrogen bond. This data item is a pointer to _atom_site.label_seq_id in the ATOM_SITE category.

**_geom_hbond.atom_site_label_seq_id_D**
An optional identifier of the donor-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_hbond.atom_site_label_seq_id_H**
An optional identifier of the hydrogen-atom site that defines the hydrogen bond. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_hbond.dist_DA** (*float, su*)
***_geom_hbond_distance_DA*** (*cif_core.dic 2.0.1*)
The distance in ångströms between the donor- and acceptor-atom sites in a hydrogen bond.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_hbond.dist_DA_esd** (associated esd). **[geom_hbond]**

**_geom_hbond.dist_DA_esd** (*float*)
The standard uncertainty (estimated standard deviation) in ångströms of **_geom_hbond.dist_DA**.
Related item: **_geom_hbond.dist_DH** (associated value). **[geom_hbond]**

**_geom_hbond.dist_DH** (*float, su*)
***_geom_hbond_distance_DH*** (*cif_core.dic 2.0.1*)
The distance in ångströms between the donor- and hydrogen-atom sites in a hydrogen bond.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_hbond.dist_DH_esd** (associated esd). **[geom_hbond]**

**_geom_hbond.dist_DH_esd** (*float*)
The standard uncertainty (estimated standard deviation) in ångströms of **_geom_hbond.dist_DH**.
Related item: **_geom_hbond.dist_DH** (associated value). **[geom_hbond]**

**_geom_hbond.dist_HA** (*float, su*)
***_geom_hbond_distance_HA*** (*cif_core.dic 2.0.1*)
The distance in ångströms between the hydrogen- and acceptor-atom sites in a hydrogen bond.
The permitted range is $[0.0, \infty)$.
Related item: **_geom_hbond.dist_HA_esd** (associated esd). **[geom_hbond]**

**_geom_hbond.dist_HA_esd** (*float*)
The standard uncertainty (estimated standard deviation) in ångströms of **_geom_hbond.dist_HA**.
Related item: **_geom_hbond.dist_HA** (associated value). **[geom_hbond]**

**_geom_hbond.publ_flag** (*ucode*)
***_geom_hbond_publ_flag*** (*cif_core.dic 2.0.1*)
This code signals whether the hydrogen-bond information is referred to in a publication or should be placed in a table of significant hydrogen-bond geometry.
The data value must be one of the following:

| | |
|---|---|
| no | do not include bond in special list |
| n | abbreviation for 'no' |
| yes | do include bond in special list |
| y | abbreviation for 'yes' |

**[geom_hbond]**

***_geom_hbond.site_symmetry_A** (*symop*)
***_geom_hbond_site_symmetry_A*** (*cif_core.dic 2.0.1*)
The symmetry code of the acceptor-atom site that defines the hydrogen bond.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_hbond]**

***_geom_hbond.site_symmetry_D** (*symop*)
***_geom_hbond_site_symmetry_D*** (*cif_core.dic 2.0.1*)
The symmetry code of the donor-atom site that defines the hydrogen bond.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_hbond]**

***_geom_hbond.site_symmetry_H** (*symop*)
***_geom_hbond_site_symmetry_H*** (*cif_core.dic 2.0.1*)
The symmetry code of the hydrogen-atom site that defines the hydrogen bond.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_hbond]**

## GEOM_TORSION

Data items in the GEOM_TORSION category record details about torsion angles as calculated from the contents of the ATOM, CELL and SYMMETRY data. The vector direction **_geom_torsion.atom_site_id_2** to **_geom_torsion.atom_site_id_3** is the viewing direction, and the torsion angle is the angle of twist required to superimpose the projection of the vector between site 2 and site 1 onto the projection of the vector between site 3 and site 4. Clockwise torsions are positive, anticlockwise torsions are negative.

Reference: Klyne, W. & Prelog, V. (1960). *Experientia*, **16**, 521–523.

Category group(s): **inclusive_group**
**geom_group**
Category key(s): **_geom_torsion.atom_site_id_1**
**_geom_torsion.atom_site_id_2**
**_geom_torsion.atom_site_id_3**
**_geom_torsion.atom_site_id_4**
**_geom_torsion.site_symmetry_1**
**_geom_torsion.site_symmetry_2**
**_geom_torsion.site_symmetry_3**
**_geom_torsion.site_symmetry_4**

*Example 1 – based on data set CLPHO6 of Ferguson, Ruhl, McKervey & Browne [Acta Cryst. (1992), C**48**, 2262–2264].*

```
loop_
_geom_torsion.atom_site_id_1
_geom_torsion.atom_site_id_2
_geom_torsion.atom_site_id_3
_geom_torsion.atom_site_id_4
_geom_torsion.value
_geom_torsion.site_symmetry_1
_geom_torsion.site_symmetry_2
_geom_torsion.site_symmetry_3
_geom_torsion.site_symmetry_4
_geom_torsion.publ_flag
 C(9)   O(2)    C(7)    C(2)     71.8  .  .  .  .      yes
 C(7)   O(2)    C(9)    C(10)  -168.0  .  .  .  2_666  yes
 C(10)  O(3)    C(8)    C(6)   -167.7  .  .  .  .      yes
 C(8)   O(3)    C(10)   C(9)    -69.7  .  .  .  2_666  yes
 O(1)   C(1)    C(2)    C(3)   -179.5  .  .  .  .      no
 O(1)   C(1)    C(2)    C(7)     -0.6  .  .  .  .      no
```

**_geom_torsion.atom_site_auth_asym_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_asym_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_asym_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_asym_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_atom_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_atom_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_atom_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_atom_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_comp_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_comp_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_comp_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_comp_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_seq_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_seq_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_seq_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_auth_seq_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_geom_torsion.atom_site_id_1**
***_geom_torsion_atom_site_label_1*** (*cif_core.dic 2.0.1*)
The identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_torsion.atom_site_id_2**
***_geom_torsion_atom_site_label_2*** (*cif_core.dic 2.0.1*)
The identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_torsion.atom_site_id_3**
***_geom_torsion_atom_site_label_3*** (*cif_core.dic 2.0.1*)
The identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

* **_geom_torsion.atom_site_id_4**
***_geom_torsion_atom_site_label_4*** (*cif_core.dic 2.0.1*)
The identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_alt_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_alt_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_alt_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_alt_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_alt_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_asym_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_asym_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_asym_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_asym_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_atom_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_atom_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_atom_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_atom_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_comp_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_comp_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_comp_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_comp_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_seq_id_1**
An optional identifier of the first of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_seq_id_2**
An optional identifier of the second of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_seq_id_3**
An optional identifier of the third of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_torsion.atom_site_label_seq_id_4**
An optional identifier of the fourth of the four atom sites that define the torsion angle. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_geom_torsion.publ_flag** (*ucode*)
***_geom_torsion_publ_flag*** (*cif_core.dic 2.0.1*)
This code signals whether the torsion angle is referred to in a publication or should be placed in a table of significant torsion angles.
The data value must be one of the following:

| | |
|---|---|
| no | do not include angle in special list |
| n | abbreviation for 'no' |
| yes | do include angle in special list |
| y | abbreviation for 'yes' |

**[geom_torsion]**

***_geom_torsion.site_symmetry_1** (*symop*)
***_geom_torsion_site_symmetry_1*** (*cif_core.dic 2.0.1*)
The symmetry code of the first of the four atom sites that define the torsion angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_torsion]**

***_geom_torsion.site_symmetry_2** (*symop*)
***_geom_torsion_site_symmetry_2*** (*cif_core.dic 2.0.1*)
The symmetry code of the second of the four atom sites that define the torsion angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_torsion]**

***_geom_torsion.site_symmetry_3** (*symop*)
***_geom_torsion_site_symmetry_3*** (*cif_core.dic 2.0.1*)
The symmetry code of the third of the four atom sites that define the torsion angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_torsion]**

***_geom_torsion.site_symmetry_4** (*symop*)
***_geom_torsion_site_symmetry_4*** (*cif_core.dic 2.0.1*)
The symmetry code of the fourth of the four atom sites that define the torsion angle.
Where no value is given, the assumed value is '1_555'.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[geom_torsion]**

**_geom_torsion.value** (*float, su*)
***_geom_torsion*** (*cif_core.dic 2.0.1*)
The value of the torsion angle in degrees.
Related item: **_geom_torsion.value_esd** (associated esd). **[geom_torsion]**

**_geom_torsion.value_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_geom_torsion.value**.
Related item: **_geom_torsion.value** (associated value). **[geom_torsion]**

## JOURNAL

Data items in the JOURNAL category record details about the book-keeping by the journal staff when processing a data block submitted for publication. The creator of a data block will not normally specify these data. The data names are not defined in the dictionary because they are for journal use only.
Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_journal.entry_id**

*Example 1 – based on Acta Cryst. file for entry HL0007 [Willis, Beckwith & Tozer (1991). Acta Cryst. C47, 2276–2277].*

```
_journal.entry_id                 'TOZ'
_journal.date_recd_electronic     1991-04-15
_journal.date_from_coeditor       1991-04-18
_journal.date_accepted            1991-04-18
_journal.date_printers_first      1991-08-07
_journal.date_proofs_out          1991-08-07
_journal.coeditor_code            HL0007
_journal.techeditor_code          C910963
_journal.coden_ASTM               ACSCEE
_journal.name_full     'Acta Crystallographica Section C'
_journal.year                     1991
_journal.volume                   47
_journal.issue                    NOV91
_journal.page_first               2276
_journal.page_last                2277
```

**_journal.coden_ASTM** (*line*)
***_journal_coden_ASTM*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coden_Cambridge** (*line*)
***_journal_coden_Cambridge*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_address** (*text*)
***_journal_coeditor_address*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_code** (*line*)
***_journal_coeditor_code*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_email** (*line*)
***_journal_coeditor_email*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_fax** (*line*)
***_journal_coeditor_fax*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_name** (*line*)
***_journal_coeditor_name*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_notes** (*text*)
***_journal_coeditor_notes*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.coeditor_phone** (*line*)
***_journal_coeditor_phone*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.data_validation_number** (*code*)
***_journal_data_validation_number*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_accepted** (*yyyy-mm-dd*)
***_journal_date_accepted*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_from_coeditor** (*yyyy-mm-dd*)
***_journal_date_from_coeditor*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_printers_final** (*yyyy-mm-dd*)
***_journal_date_printers_final*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_printers_first** (*yyyy-mm-dd*)
***_journal_date_printers_first*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_proofs_in** (*yyyy-mm-dd*)
***_journal_date_proofs_in*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_proofs_out** (*yyyy-mm-dd*)
***_journal_date_proofs_out*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff. **[journal]**

**_journal.date_recd_copyright** (*yyyy-mm-dd*)
***_journal_date_recd_copyright*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.date_recd_electronic** (*yyyy-mm-dd*)
***_journal_date_recd_electronic*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.date_recd_hard_copy** (*yyyy-mm-dd*)
***_journal_date_recd_hard_copy*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.date_to_coeditor** (*yyyy-mm-dd*)
***_journal_date_to_coeditor*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

* **_journal.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_journal.issue** (*line*)
***_journal_issue*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.language** (*line*)
***_journal_language*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.name_full** (*line*)
***_journal_name_full*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.page_first** (*line*)
***_journal_page_first*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.page_last** (*line*)
***_journal_page_last*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.paper_category** (*line*)
***_journal_paper_category*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.suppl_publ_number** (*line*)
***_journal_suppl_publ_number*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.suppl_publ_pages** (*line*)
***_journal_suppl_publ_pages*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_address** (*text*)
***_journal_techeditor_address*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_code** (*line*)
***_journal_techeditor_code*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_email** (*line*)
***_journal_techeditor_email*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_fax** (*line*)
***_journal_techeditor_fax*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_name** (*line*)
***_journal_techeditor_name*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_notes** (*text*)
***_journal_techeditor_notes*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.techeditor_phone** (*line*)
***_journal_techeditor_phone*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.volume** (*line*)
***_journal_volume*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

**_journal.year** (*line*)
***_journal_year*** (*cif_core.dic 2.0.1*)
Journal data items are defined by the journal staff.
**[journal]**

## JOURNAL_INDEX

Data items in the JOURNAL_INDEX category are used to list terms used to generate the journal indexes. The creator of a data block will not normally specify these data items.

Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_journal_index.type**
**_journal_index.term**

*Example 1 – based on a paper by Zhu, Reynolds, Klein & Trudell [Acta Cryst. (1994), **C50**, 2067–2069].*

```
loop_
_journal_index.type
_journal_index.term
_journal_index.subterm
  O   C16H19NO4            .
  S   alkaloids           (-)-norcocaine
  S   (-)-norcocaine       .
  S
;  [2R,3S-(2\b,3\b)]-methyl
   3-(benzoyloxy)-8-azabicyclo[3.2.1]octane-2-carboxylate
;
       .
```

**_journal_index.subterm** (*line*)
***_journal_index_subterm*** (*cif_core.dic 2.0.1*)
Journal index data items are defined by the journal staff.
**[journal_index]**

**_journal_index.term** (*line*)
***_journal_index_term*** (*cif_core.dic 2.0.1*)
Journal index data items are defined by the journal staff.
**[journal_index]**

**_journal_index.type** (*line*)
***_journal_index_type*** (*cif_core.dic 2.0.1*)
Journal index data items are defined by the journal staff.

**[journal_index]**

## PHASING

Data items in the PHASING category record details about the phasing of the structure, listing the various methods used in the phasing process. Details about the application of each method are listed in the appropriate subcategories.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing.method**

*Example 1 – hypothetical example.*

```
loop_
_phasing.method
'mir'
'averaging'
```

* **_phasing.method** (*ucode*)
A listing of the method or methods used to phase this structure.
Examples: 'abinitio' (phasing by *ab initio* methods), 'averaging' (phase improvement by averaging over multiple images of the structure), 'dm' (phasing by direct methods), 'isas' (phasing by iterative single-wavelength anomalous scattering), 'isir' (phasing by iterative single-wavelength isomorphous replacement), 'isomorphous' (phasing beginning with phases calculated from an isomorphous structure), 'mad' (phasing by multiple-wavelength anomalous dispersion), 'mir' (phasing by multiple isomorphous replacement), 'miras' (phasing by multiple isomorphous replacement with anomalous scattering), 'mr' (phasing by molecular replacement), 'sir' (phasing by single isomorphous replacement), 'siras' (phasing by single isomorphous replacement with anomalous scattering). **[phasing]**

## PHASING_AVERAGING

Data items in the PHASING_AVERAGING category record details about the phasing of the structure where methods involving averaging of multiple observations of the molecule in the asymmetric unit are involved.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_averaging.entry_id**

*Example 1 – hypothetical example.*

```
_phasing_averaging.entry_id    'EXAMHYPO'
_phasing_averaging.method
; Iterative threefold averaging alternating with phase
  extensions by 0.5 reciprocal lattice units per cycle.
;
_phasing_averaging.details
; The position of the threefold axis was redetermined every
  five cycles.
;
```

**_phasing_averaging.details** (*text*)
A description of special aspects of the averaging process.

**[phasing_averaging]**

* **_phasing_averaging.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_phasing_averaging.method** (*text*)
A description of the phase-averaging phasing method used to phase this structure. Note that this is not the computer program used, which is described in the SOFTWARE category, but rather the method itself. This data item should be used to describe significant methodological options used within the phase-averaging program.

**[phasing_averaging]**

## PHASING_ISOMORPHOUS

Data items in the PHASING_ISOMORPHOUS category record details about the phasing of the structure where a model isomorphous to the structure being phased was used to generate the initial phases.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_isomorphous.entry_id**

*Example 1 – based on PDB entry 4PHV and laboratory records for the structure corresponding to PDB entry 4PHV.*

```
_phasing_isomorphous.parent           'PDB entry 5HVP'
_phasing_isomorphous.details
; The inhibitor and all solvent atoms were removed from the
  parent structure before beginning refinement. All static
  disorder present in the parent structure was also removed.
;
```

**_phasing_isomorphous.details** (*text*)
A description of special aspects of the isomorphous phasing.
Example:

```
; Residues 13-18 were eliminated from the starting model as it
was anticipated that binding of the inhibitor would cause a
structural rearrangement in this part of the structure.
;
```

**[phasing_isomorphous]**

* **_phasing_isomorphous.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_phasing_isomorphous.method** (*text*)
A description of the isomorphous-phasing method used to phase this structure. Note that this is not the computer program used, which is described in the SOFTWARE category, but rather the method itself. This data item should be used to describe significant methodological options used within the isomorphous phasing program.
Example:

```
; Iterative threefold averaging alternating with phase
extension by 0.5 reciprocal lattice units per cycle.
;
```

**[phasing_isomorphous]**

**_phasing_isomorphous.parent** (*text*)
Reference to the structure used to generate starting phases if the structure referenced in this data block was phased by virtue of being isomorphous to a known structure (*e.g.* a mutant that crystallizes in the same space group as the wild-type protein.)

**[phasing_isomorphous]**

## PHASING_MAD

Data items in the PHASING_MAD category record details about the phasing of the structure where methods involving multiple-wavelength anomalous-dispersion techniques are involved.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MAD.entry_id**

*Example 1 – based on a paper by Shapiro et al. [Nature (London) (1995), **374**, 327–337].*

```
_phasing_MAD.entry_id       'NCAD'
```

**_phasing_MAD.details** (*text*)
A description of special aspects of the MAD phasing.

**[phasing_MAD]**

* **_phasing_MAD.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_phasing_MAD.method** (*text*)
A description of the MAD phasing method used to phase this structure. Note that this is not the computer program used, which is described in the SOFTWARE category, but rather the method itself. This data item should be used to describe significant methodological options used within the MAD phasing program.

[phasing_MAD]

## PHASING_MAD_CLUST

Data items in the PHASING_MAD_CLUST category record details about a cluster of experiments that contributed to the generation of a set of phases.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MAD_clust.expt_id**
**_phasing_MAD_clust.id**

*Example 1 – based on a paper by Shapiro et al. [Nature (London) (1995), **374**, 327–337].*

```
loop_
_phasing_MAD_clust.id
_phasing_MAD_clust.expt_id
_phasing_MAD_clust.number_set
  '4 wavelength'  1  4
  '5 wavelength'  1  5
  '5 wavelength'  2  5
```

* **_phasing_MAD_clust.expt_id**
This data item is a pointer to **_phasing_MAD_expt.id** in the PHASING_MAD_EXPT category.

* **_phasing_MAD_clust.id** (*code*)
The value of **_phasing_MAD_clust.id** must, together with **_phasing_MAD_clust.expt_id**, uniquely identify a record in the PHASING_MAD_CLUST list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*
***_phasing_MAD_set.clust_id***,
***_phasing_MAD_ratio.clust_id***. [phasing_MAD_clust]

**_phasing_MAD_clust.number_set** (*int*)
The number of data sets in this cluster of data sets.

[phasing_MAD_clust]

## PHASING_MAD_EXPT

Data items in the PHASING_MAD_EXPT category record details about a MAD phasing experiment, such as the number of experiments that were clustered together to produce a set of phases or the statistics for those phases.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MAD_expt.id**

*Example 1 – based on a paper by Shapiro et al. [Nature (London) (1995), **374**, 327–337].*

```
loop_
_phasing_MAD_expt.id
_phasing_MAD_expt.number_clust
_phasing_MAD_expt.R_normal_all
_phasing_MAD_expt.R_normal_anom_scat
_phasing_MAD_expt.delta_delta_phi
_phasing_MAD_expt.delta_phi_sigma
_phasing_MAD_expt.mean_fom
  1  2  0.063  0.451  58.5  20.3  0.88
  2  1  0.051  0.419  36.8  18.2  0.93
```

**_phasing_MAD_expt.delta_delta_phi** (*float*)
The difference between two independent determinations of **_phasing_MAD_expt.delta_phi**.

[phasing_MAD_expt]

**_phasing_MAD_expt.delta_phi** (*float*)
The phase difference between $F_t(h)$, the structure factor due to normal scattering from all atoms, and $F_a(h)$, the structure factor due to normal scattering from only the anomalous scatterers.

Related item: **_phasing_MAD_expt.delta_phi_sigma** (associated esd).

[phasing_MAD_expt]

**_phasing_MAD_expt.delta_phi_sigma** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MAD_expt.delta_phi**.

Related item: **_phasing_MAD_expt.delta_phi** (associated value).

[phasing_MAD_expt]

* **_phasing_MAD_expt.id** (*code*)
The value of **_phasing_MAD_expt.id** must uniquely identify each record in the PHASING_MAD_EXPT list.

*The following item(s) have an equivalent role in their respective categories:*
***_phasing_MAD_clust.expt_id***,
***_phasing_MAD_set.expt_id***,
***_phasing_MAD_ratio.expt_id***. [phasing_MAD_expt]

**_phasing_MAD_expt.mean_fom** (*float*)
The mean figure of merit.

[phasing_MAD_expt]

**_phasing_MAD_expt.number_clust** (*int*)
The number of clusters of data sets in this phasing experiment.

[phasing_MAD_expt]

**_phasing_MAD_expt.R_normal_all** (*float*)

[phasing_MAD_expt]

**_phasing_MAD_expt.R_normal_anom_scat** (*float*)

[phasing_MAD_expt]

## PHASING_MAD_RATIO

Data items in the PHASING_MAD_RATIO category record the ratios of phasing statistics between pairs of data sets in a MAD phasing experiment, in given shells of resolution.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MAD_ratio.clust_id**
**_phasing_MAD_ratio.expt_id**
**_phasing_MAD_ratio.wavelength_1**
**_phasing_MAD_ratio.wavelength_2**

*Example 1 – based on a paper by Shapiro et al. [Nature (London) (1995), **374**, 327–337].*

```
loop_
_phasing_MAD_ratio.expt_id
_phasing_MAD_ratio.clust_id
_phasing_MAD_ratio.wavelength_1
_phasing_MAD_ratio.wavelength_2
_phasing_MAD_ratio.d_res_low
_phasing_MAD_ratio.d_res_high
_phasing_MAD_ratio.ratio_two_wl
_phasing_MAD_ratio.ratio_one_wl
_phasing_MAD_ratio.ratio_one_wl_centric
 1 '4 wavelength' 1.4013 1.4013 20.00 4.00     . 0.084 0.076
 1 '4 wavelength' 1.4013 1.3857 20.00 4.00 0.067     .     .
 1 '4 wavelength' 1.4013 1.3852 20.00 4.00 0.051     .     .
 1 '4 wavelength' 1.4013 1.3847 20.00 4.00 0.044     .     .
 1 '4 wavelength' 1.3857 1.3857 20.00 4.00     . 0.110 0.049
 1 '4 wavelength' 1.3857 1.3852 20.00 4.00 0.049     .     .
 1 '4 wavelength' 1.3857 1.3847 20.00 4.00 0.067     .     .
 1 '4 wavelength' 1.3852 1.3852 20.00 4.00     . 0.149 0.072
 1 '4 wavelength' 1.3852 1.3847 20.00 4.00 0.039     .     .
 1 '4 wavelength' 1.3847 1.3847 20.00 4.00     . 0.102 0.071

 1 '4 wavelength' 1.4013 1.4013  4.00 3.00     . 0.114 0.111
 1 '4 wavelength' 1.4013 1.3857  4.00 3.00 0.089     .     .
 1 '4 wavelength' 1.4013 1.3852  4.00 3.00 0.086     .     .
 1 '4 wavelength' 1.4013 1.3847  4.00 3.00 0.077     .     .
 1 '4 wavelength' 1.3857 1.3857  4.00 3.00     . 0.140 0.127
 1 '4 wavelength' 1.3857 1.3852  4.00 3.00 0.085     .     .
 1 '4 wavelength' 1.3857 1.3847  4.00 3.00 0.089     .     .
 1 '4 wavelength' 1.3852 1.3852  4.00 3.00     . 0.155 0.119
 1 '4 wavelength' 1.3852 1.3847  4.00 3.00 0.082     .     .
 1 '4 wavelength' 1.3847 1.3847  4.00 3.00     . 0.124 0.120

 1 '5 wavelength' 1.3857 1.3857 20.00 4.00     . 0.075 0.027
 1 '5 wavelength' 1.3857 1.3852 20.00 4.00 0.041     .     .
 1 '5 wavelength' 1.3857 1.3847 20.00 4.00 0.060     .     .
 1 '5 wavelength' 1.3857 1.3784 20.00 4.00 0.057     .     .
 1 '5 wavelength' 1.3857 1.2862 20.00 4.00 0.072     .     .
 1 '5 wavelength' 1.3852 1.3852 20.00 4.00     . 0.105 0.032
 1 '5 wavelength' 1.3852 1.3847 20.00 4.00 0.036     .     .
 1 '5 wavelength' 1.3852 1.3784 20.00 4.00 0.044     .     .
 1 '5 wavelength' 1.3852 1.2862 20.00 4.00 0.065     .     .
 1 '5 wavelength' 1.3847 1.3847 20.00 4.00     . 0.072 0.031
 1 '5 wavelength' 1.3847 1.3784 20.00 4.00 0.040     .     .
 1 '5 wavelength' 1.3847 1.2862 20.00 4.00 0.059     .     .
 1 '5 wavelength' 1.3784 1.3784 20.00 4.00     . 0.059 0.032
 1 '5 wavelength' 1.3784 1.2862 20.00 4.00 0.059     .     .
 1 '5 wavelength' 1.2862 1.3847 20.00 4.00     . 0.058 0.028

 1 '5 wavelength' 1.3857 1.3857  4.00 3.00     . 0.078 0.075
 1 '5 wavelength' 1.3857 1.3852  4.00 3.00 0.059     .     .
 1 '5 wavelength' 1.3857 1.3847  4.00 3.00 0.067     .     .
 1 '5 wavelength' 1.3857 1.3784  4.00 3.00 0.084     .     .
 1 '5 wavelength' 1.3857 1.2862  4.00 3.00 0.073     .     .
 1 '5 wavelength' 1.3852 1.3852  4.00 3.00     . 0.101 0.088
 1 '5 wavelength' 1.3852 1.3847  4.00 3.00 0.066     .     .
 1 '5 wavelength' 1.3852 1.3784  4.00 3.00 0.082     .     .
 1 '5 wavelength' 1.3852 1.2862  4.00 3.00 0.085     .     .
 1 '5 wavelength' 1.3847 1.3847  4.00 3.00     . 0.097 0.074
 1 '5 wavelength' 1.3847 1.3784  4.00 3.00 0.081     .     .
 1 '5 wavelength' 1.3847 1.2862  4.00 3.00 0.085     .     .
 1 '5 wavelength' 1.3784 1.3784  4.00 3.00     . 0.114 0.089
 1 '5 wavelength' 1.3784 1.2862  4.00 3.00 0.103     .     .
 1 '5 wavelength' 1.2862 1.2862  4.00 3.00     . 0.062 0.060

 2 '5 wavelength' 0.7263 0.7263 15.00 3.00     . 0.035 0.026
 2 '5 wavelength' 0.7263 0.7251 15.00 3.00 0.028     .     .
 2 '5 wavelength' 0.7263 0.7284 15.00 3.00 0.023     .     .
 2 '5 wavelength' 0.7263 0.7246 15.00 3.00 0.025     .     .
 2 '5 wavelength' 0.7263 0.7217 15.00 3.00 0.026     .     .
 2 '5 wavelength' 0.7251 0.7251 15.00 3.00     . 0.060 0.026
 2 '5 wavelength' 0.7251 0.7284 15.00 3.00 0.029     .     .
 2 '5 wavelength' 0.7251 0.7246 15.00 3.00 0.031     .     .
 2 '5 wavelength' 0.7251 0.7217 15.00 3.00 0.035     .     .
 2 '5 wavelength' 0.7284 0.7284 15.00 3.00     . 0.075 0.030
 2 '5 wavelength' 0.7284 0.7246 15.00 3.00 0.023     .     .
 2 '5 wavelength' 0.7284 0.7217 15.00 3.00 0.027     .     .
 2 '5 wavelength' 0.7246 0.7246 15.00 3.00     . 0.069 0.026
 2 '5 wavelength' 0.7246 0.7217 15.00 3.00 0.024     .     .
 2 '5 wavelength' 0.7217 0.7284 15.00 3.00     . 0.060 0.028

 2 '5 wavelength' 0.7263 0.7263  3.00 1.90     . 0.060 0.050
 2 '5 wavelength' 0.7263 0.7251  3.00 1.90 0.056     .     .
 2 '5 wavelength' 0.7263 0.7284  3.00 1.90 0.055     .     .
 2 '5 wavelength' 0.7263 0.7246  3.00 1.90 0.053     .     .
 2 '5 wavelength' 0.7263 0.7217  3.00 1.90 0.056     .     .
 2 '5 wavelength' 0.7251 0.7251  3.00 1.90     . 0.089 0.050
 2 '5 wavelength' 0.7251 0.7284  3.00 1.90 0.054     .     .
 2 '5 wavelength' 0.7251 0.7246  3.00 1.90 0.058     .     .
 2 '5 wavelength' 0.7251 0.7217  3.00 1.90 0.063     .     .
 2 '5 wavelength' 0.7284 0.7284  3.00 1.90     . 0.104 0.057
 2 '5 wavelength' 0.7284 0.7246  3.00 1.90 0.052     .     .
 2 '5 wavelength' 0.7284 0.7217  3.00 1.90 0.057     .     .
 2 '5 wavelength' 0.7246 0.7246  3.00 1.90     . 0.098 0.052
 2 '5 wavelength' 0.7246 0.7217  3.00 1.90 0.054     .     .
 2 '5 wavelength' 0.7217 0.7284  3.00 1.90     . 0.089 0.060
```

* **_phasing_MAD_ratio.clust_id**
This data item is a pointer to **_phasing_MAD_clust.id** in the PHASING_MAD_CLUST category.

**_phasing_MAD_ratio.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data used for the comparison of Bijvoet differences. This is called the highest resolution.

**[phasing_MAD_ratio]**

**_phasing_MAD_ratio.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data used for the comparison of Bijvoet differences. This is called the lowest resolution.

**[phasing_MAD_ratio]**

* **_phasing_MAD_ratio.expt_id**
This data item is a pointer to **_phasing_MAD_expt.id** in the PHASING_MAD_EXPT category.

**_phasing_MAD_ratio.ratio_one_wl** (*float*)
The root-mean-square Bijvoet difference at one wavelength for all reflections.

**[phasing_MAD_ratio]**

**_phasing_MAD_ratio.ratio_one_wl_centric** (*float*)
The root-mean-square Bijvoet difference at one wavelength for centric reflections. This would be equal to zero for perfect data and thus serves as an estimate of the noise in the anomalous signals.

**[phasing_MAD_ratio]**

**_phasing_MAD_ratio.ratio_two_wl** (*float*)
The root-mean-square dispersive Bijvoet difference between two wavelengths for all reflections.

**[phasing_MAD_ratio]**

* **_phasing_MAD_ratio.wavelength_1**
This data item is a pointer to **_phasing_MAD_set.wavelength** in the PHASING_MAD_SET category.

* **_phasing_MAD_ratio.wavelength_2**
This data item is a pointer to **_phasing_MAD_set.wavelength** in the PHASING_MAD_SET category.

## PHASING_MAD_SET

Data items in the PHASING_MAD_SET category record details about the individual data sets used in a MAD phasing experiment.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MAD_set.expt_id**
**_phasing_MAD_set.clust_id**
**_phasing_MAD_set.set_id**
**_phasing_MAD_set.wavelength**

*Example 1 – based on a paper by Shapiro et al. [Nature (London) (1995), **374**, 327–337].*

```
loop_
_phasing_MAD_set.expt_id
_phasing_MAD_set.clust_id
_phasing_MAD_set.set_id
_phasing_MAD_set.wavelength
_phasing_MAD_set.wavelength_details
_phasing_MAD_set.d_res_low
_phasing_MAD_set.d_res_high
_phasing_MAD_set.f_prime
_phasing_MAD_set.f_double_prime
1 '4 wavelength' aa 1.4013 'pre-edge'         20.00   3.00
     -12.48   3.80
1 '4 wavelength' bb 1.3857 'peak'            20.00   3.00
     -31.22  17.20
1 '4 wavelength' cc 1.3852 'edge'             20.00   3.00
     -13.97  29.17
1 '4 wavelength' dd 1.3847 'remote'           20.00   3.00
     -6.67  17.34
1 '5 wavelength' ee 1.3857 'ascending edge'   20.00   3.00
     -28.33  14.84
1 '5 wavelength' ff 1.3852 'peak'             20.00   3.00
     -21.50  30.23
1 '5 wavelength' gg 1.3847 'descending edge' 20.00   3.00
     -10.71  20.35
1 '5 wavelength' hh 1.3784 'remote 1'         20.00   3.00
     -14.45  11.84
1 '5 wavelength' ii 1.2862 'remote 2'         20.00   3.00
     -9.03   9.01
2 '5 wavelength' jj 0.7263 'pre-edge'         15.00   1.90
     -21.10   4.08
2 '5 wavelength' kk 0.7251 'edge'             15.00   1.90
     -34.72   7.92
2 '5 wavelength' ll 0.7248 'peak'             15.00   1.90
     -24.87  10.30
2 '5 wavelength' mm 0.7246 'descending edge' 15.00   1.90
     -17.43   9.62
2 '5 wavelength' nn 0.7217 'remote'           15.00   1.90
     -13.26   8.40
```

* **_phasing_MAD_set.clust_id**
This data item is a pointer to **_phasing_MAD_clust.id** in the PHASING_MAD_CLUST category.

**_phasing_MAD_set.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data used for this set of data. This is called the highest resolution.
**[phasing_MAD_set]**

**_phasing_MAD_set.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data used for this set of data. This is called the lowest resolution.
**[phasing_MAD_set]**

* **_phasing_MAD_set.expt_id**
This data item is a pointer to **_phasing_MAD_expt.id** in the PHASING_MAD_EXPT category.

**_phasing_MAD_set.f_double_prime** (*float*)
The $f''$ component of the anomalous scattering factor for this wavelength.
**[phasing_MAD_set]**

**_phasing_MAD_set.f_prime** (*float*)
The $f'$ component of the anomalous scattering factor for this wavelength.
**[phasing_MAD_set]**

* **_phasing_MAD_set.set_id**
This data item is a pointer to **_phasing_set.id** in the PHASING_SET category.

* **_phasing_MAD_set.wavelength** (*float*)
The wavelength at which this data set was measured.
*The following item(s) have an equivalent role in their respective categories:*
***_phasing_MAD_ratio.wavelength_1***,
***_phasing_MAD_ratio.wavelength_2***. **[phasing_MAD_set]**

**_phasing_MAD_set.wavelength_details** (*text*)
A descriptor for this wavelength in this cluster of data sets.
Examples: 'peak', 'remote', 'ascending edge'. **[phasing_MAD_set]**

## PHASING_MIR

Data items in the PHASING_MIR category record details about the phasing of the structure where methods involving isomorphous replacement are involved. All isomorphous-replacement-based techniques are covered by this category, including single isomorphous replacement (SIR), multiple isomorphous replacement (MIR) and single or multiple isomorphous replacement plus anomalous scattering (SIRAS, MIRAS).

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR.entry_id**

*Example 1 – based on a paper by Zanotti et al. [J. Biol. Chem. (1993), **268**, 10728–10738].*

```
_phasing_MIR.method
; Standard phase refinement (Blow & Crick, 1959)
;
```

* **_phasing_MIR.d_res_high** (*float*)
***_phasing_MIR.ebi_d_res_high*** (*ebi_extensions 1.0*)
The lowest value in ångströms for the interplanar spacings for the reflection data used for the native data set. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR]**

* **_phasing_MIR.d_res_low** (*float*)
***_phasing_MIR.ebi_d_res_low*** (*ebi_extensions 1.0*)
The highest value in ångströms for the interplanar spacings for the reflection data used for the native data set. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.details** (*text*)
A description of special aspects of the isomorphous-replacement phasing.
**[phasing_MIR]**

* **_phasing_MIR.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_phasing_MIR.FOM** (*float*)
***_phasing_MIR.ebi_fom*** (*ebi_extensions 1.0*)
The mean value of the figure of merit *m* for all reflections phased in the native data set.

$$m = \frac{\int P_\alpha \exp(i\alpha)\, \mathrm{d}\alpha}{\int P_\alpha \, \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.FOM_acentric** (*float*)
***_phasing_MIR.ebi_fom_acentric*** (*ebi_extensions 1.0*)
The mean value of the figure of merit *m* for the acentric reflections phased in the native data set.

$$m = \frac{\int P_\alpha \exp(i\alpha)\, \mathrm{d}\alpha}{\int P_\alpha \, \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.FOM_centric** (*float*)
***_phasing_MIR.ebi_fom_centric*** (*ebi_extensions 1.0*)
The mean value of the figure of merit *m* for the centric reflections phased in the native data set.

$$m = \frac{\int P_\alpha \exp(i\alpha)\, \mathrm{d}\alpha}{\int P_\alpha \, \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.method** (*text*)
A description of the MIR phasing method applied to phase this structure. Note that this is not the computer program used, which is described in the SOFTWARE category, but rather the method itself. This data item should be used to describe significant methodological options used within the MIR phasing program.
**[phasing_MIR]**

**_phasing_MIR.reflns** (*int*)
***_phasing_MIR.ebi_reflns*** (*ebi_extensions 1.0*)
The total number of reflections phased in the native data set.
The permitted range is $[0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.reflns_acentric** (*int*)
***_phasing_MIR.ebi_reflns_acentric*** (*ebi_extensions 1.0*)
The number of acentric reflections phased in the native data set.
The permitted range is $[0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.reflns_centric** (*int*)
***_phasing_MIR.ebi_reflns_centric*** (*ebi_extensions 1.0*)
The number of centric reflections phased in the native data set.
The permitted range is $[0, \infty)$. **[phasing_MIR]**

**_phasing_MIR.reflns_criterion** (*text*)
***_phasing_MIR.ebi_reflns_criteria*** (*ebi_extensions 1.0*)
Criterion used to limit the reflections used in the phasing calculations.
Example: '`> 4 \s(I)`'. **[phasing_MIR]**

## PHASING_MIR_DER

Data items in the PHASING_MIR_DER category record details about individual derivatives used in the phasing of the structure when methods involving isomorphous replacement are involved. A derivative in this context does not necessarily equate with a data set; for instance, the same data set could be used to one resolution limit as an isomorphous scatterer and to a different resolution (and with a different $\sigma$ cut-off) as an anomalous scatterer. These would be treated as two distinct derivatives, although both derivatives would point to the same data sets *via* **_phasing_MIR_der.der_set_id** and **_phasing_MIR_der.native_set_id**.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR_der.id**

*Example 1 – based on a paper by Zanotti et al. [J. Biol. Chem. (1993), **268**, 10728–10738].*

```
loop_
_phasing_MIR_der.id
_phasing_MIR_der.number_of_sites
_phasing_MIR_der.details
KAu(CN)2  3  'major site interpreted in difference Patterson'
K2HgI4    6  'sites found in cross-difference Fourier'
K3IrCl6   2  'sites found in cross-difference Fourier'
All      11  'data for all three derivatives combined'
```

***_phasing_MIR_der.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data used for this derivative. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

***_phasing_MIR_der.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data used for this derivative. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

***_phasing_MIR_der.der_set_id**
The data set that was treated as the derivative in this experiment. This data item is a pointer to **_phasing_set.id** in the PHASING_SET category.

**_phasing_MIR_der.details** (*text*)
A description of special aspects of this derivative, its data, its solution or its use in phasing.
**[phasing_MIR_der]**

***_phasing_MIR_der.id** (*line*)
The value of **_phasing_MIR_der.id** must uniquely identify a record in the PHASING_MIR_DER list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_phasing_MIR_der_refln.der_id***,
***_phasing_MIR_der_shell.der_id***,
***_phasing_MIR_der_site.der_id***.
Examples: '`KAu(CN)2`', '`K2HgI4_anom`', '`K2HgI4_iso`'. **[phasing_MIR_der]**

***_phasing_MIR_der.native_set_id**
The data set that was treated as the native in this experiment. This data item is a pointer to **_phasing_set.id** in the PHASING_SET category.

**_phasing_MIR_der.number_of_sites** (*int*)
The number of heavy-atom sites in this derivative.
**[phasing_MIR_der]**

**_phasing_MIR_der.power_acentric** (*float*)
***_phasing_MIR_der.ebi_power_acentric*** (*ebi_extensions 1.0*)
The mean phasing power $P$ for acentric reflections for this derivative.

$$P = \left( \frac{\sum |F(h)^2_{\rm calc}|}{\sum |F(ph)_{\rm obs} - F(ph)_{\rm calc}|^2} \right)^{1/2},$$

where $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of this derivative, $F(ph)_{\rm calc}$ = the calculated structure-factor amplitude of this derivative and $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.power_centric** (*float*)
***_phasing_MIR_der.ebi_power_centric*** (*ebi_extensions 1.0*)
The mean phasing power $P$ for centric reflections for this derivative.

$$P = \left( \frac{\sum |F(h)^2_{\rm calc}|}{\sum |F(ph)_{\rm obs} - F(ph)_{\rm calc}|^2} \right)^{1/2},$$

where $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of this derivative, $F(ph)_{\rm calc}$ = the calculated structure-factor amplitude of this derivative and $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.R_cullis_acentric** (*float*)
***_phasing_MIR_der.ebi_Rcullis_acentric*** (*ebi_extensions 1.0*)
Residual factor $R_{\rm cullis,acen}$ for acentric reflections for this derivative. The Cullis $R$ factor was originally defined only for centric reflections. It is, however, also a useful statistical measure for acentric reflections, which is how it is used in this data item.

$$R_{\rm cullis,acen} = \frac{\sum \Big| |F(ph)_{\rm obs} \pm F(p)_{\rm obs}| - F(h)_{\rm calc} \Big|}{\sum |F(ph)_{\rm obs} - F(p)_{\rm obs}|},$$

where $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative and $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.

Reference: Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. London Ser. A*, **265**, 15–38.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.R_cullis_anomalous** (*float*)
***_phasing_MIR_der.ebi_Rcullis_anomalous*** (*ebi_extensions 1.0*)
Residual factor $R_{\rm cullis,ano}$ for anomalous reflections for this derivative. The Cullis $R$ factor was originally defined only for centric reflections. It is, however, also a useful statistical measure for anomalous reflections, which is how it is used in this data item. This is tabulated for acentric terms. A value less than 1.0 means there is some contribution to the phasing from the anomalous data.

$$R_{\rm cullis,ano} = \frac{\sum |F(ph+)_{\rm obs} F(ph-)_{\rm obs} - F(h+)_{\rm calc} - F(h-)_{\rm calc}|}{\sum |F(ph+)_{\rm obs} - F(ph-)_{\rm obs}|},$$

where $F(ph+)_{\rm obs}$ = the observed positive Friedel structure-factor amplitude for the derivative, $F(ph-)_{\rm obs}$ = the observed negative Friedel structure-factor amplitude for the derivative, $F(h+)_{\rm calc}$ = the calculated positive Friedel structure-factor amplitude from the heavy-atom model and $F(h-)_{\rm calc}$ = the calculated negative Friedel structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.

Reference: Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. London Ser. A*, **265**, 15–38.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.R_cullis_centric** (*float*)
***_phasing_MIR_der.ebi_Rcullis_centric*** (*ebi_extensions 1.0*)
Residual factor $R_{\rm cullis}$ for centric reflections for this derivative.

$$R_{\rm cullis} = \frac{\sum \Big| |F(ph)_{\rm obs} \pm F(p)_{\rm obs}| - F(h)_{\rm calc} \Big|}{\sum |F(ph)_{\rm obs} - F(p)_{\rm obs}|},$$

where $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative and $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.

Reference: Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. London Ser. A*, **265**, 15–38.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.reflns_acentric** (*int*)
***_phasing_MIR_der.ebi_reflns_acentric*** (*ebi_extensions 1.0*)
The number of acentric reflections used in phasing for this derivative.
The permitted range is $[0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.reflns_anomalous** (*int*)
***_phasing_MIR_der.ebi_reflns_anomalous*** (*ebi_extensions 1.0*)
The number of anomalous reflections used in phasing for this derivative.
The permitted range is $[0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.reflns_centric** (*int*)
***_phasing_MIR_der.ebi_reflns_centric*** (*ebi_extensions 1.0*)
The number of centric reflections used in phasing for this derivative.
The permitted range is $[0, \infty)$. **[phasing_MIR_der]**

**_phasing_MIR_der.reflns_criteria** (*text*)
Criteria used to limit the reflections used in the phasing calculations.
Example: '`> 4 \s(I)`'. **[phasing_MIR_der]**

## PHASING_MIR_DER_REFLN

Data items in the PHASING_MIR_DER_REFLN category record details about the calculated structure factors obtained in an MIR phasing experiment. This list may contain information from a number of different derivatives; **_phasing_MIR_der_refln.der_id** indicates to which derivative a given record corresponds. (A derivative in this context does not necessarily equate with a data set; see the definition of the PHASING_MIR_DER category for a discussion of the meaning of 'derivative'.) It is not necessary for the data items describing the measured value of $F$ to appear in this list, as they will be given in the PHASING_SET_REFLN category. However, these items can also be listed here for completeness.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR_der_refln.index_h**
**_phasing_MIR_der_refln.index_k**
**_phasing_MIR_der_refln.index_l**
**_phasing_MIR_der_refln.der_id**
**_phasing_MIR_der_refln.set_id**

*Example 1 – based on laboratory records for the 6,1,25 reflection of an Hg/Pt derivative of protein NS1.*

```
_phasing_MIR_der_refln.index_h         6
_phasing_MIR_der_refln.index_k         1
_phasing_MIR_der_refln.index_l        25
_phasing_MIR_der_refln.der_id         HGPT1
_phasing_MIR_der_refln.set_id       'NS1-96'
_phasing_MIR_der_refln.F_calc_au     106.66
_phasing_MIR_der_refln.F_meas_au     204.67
_phasing_MIR_der_refln.F_meas_sigma    6.21
_phasing_MIR_der_refln.HL_A_iso       -3.15
_phasing_MIR_der_refln.HL_B_iso       -0.76
_phasing_MIR_der_refln.HL_C_iso        0.65
_phasing_MIR_der_refln.HL_D_iso        0.23
_phasing_MIR_der_refln.phase_calc    194.48
```

* **_phasing_MIR_der_refln.der_id**
This data item is a pointer to **_phasing_MIR_der.id** in the PHASING_MIR_DER category.

**_phasing_MIR_der_refln.F_calc** (*float*)
The calculated value of the structure factor for this derivative, in electrons.
Related item: **_phasing_MIR_der_refln.F_calc_au** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.F_calc_au** (*float*)
The calculated value of the structure factor for this derivative, in arbitrary units.
Related item: **_phasing_MIR_der_refln.F_calc** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.F_meas** (*float, su*)
The measured value of the structure factor for this derivative, in electrons.
Related items: **_phasing_MIR_der_refln.F_meas_sigma** (associated esd), **_phasing_MIR_der_refln.F_meas_au** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.F_meas_au** (*float, su*)
The measured value of the structure factor for this derivative, in arbitrary units.
Related items: **_phasing_MIR_der_refln.F_meas_sigma_au** (associated esd), **_phasing_MIR_der_refln.F_meas** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.F_meas_sigma** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_refln.F_meas**, in electrons.
Related items: **_phasing_MIR_der_refln.F_meas** (associated value), **_phasing_MIR_der_refln.F_meas_sigma_au** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.F_meas_sigma_au** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_refln.F_meas_au**, in arbitrary units.
Related items: **_phasing_MIR_der_refln.F_meas_au** (associated value), **_phasing_MIR_der_refln.F_meas_sigma** (conversion arbitrary).
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.HL_A_iso** (*float*)
The isomorphous Hendrickson–Lattman coefficient $A_{\rm iso}$ for this reflection for this derivative.

$$A_{\rm iso} = -\frac{2.0[F(p)^2_{\rm obs} + F(h)^2_{\rm calc} - F(ph)^2_{\rm obs}]F(p)_{\rm obs}\cos(\alpha_{h\rm calc})}{E^2},$$

where $E = [F(ph)_{\rm obs} - F(p)_{\rm obs} - F(h)_{\rm calc}]^2$ for centric reflections, $E = \{2^{1/2}[F(ph)_{\rm obs} - F(p)_{\rm obs}] - F(h)_{\rm calc}\}^2$ for acentric reflections, $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative, $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model and $\alpha_{h\rm calc}$ = the calculated phase from the heavy-atom model.

This coefficient appears in the expression for the phase probability of each isomorphous derivative:

$$P_i(\alpha) = \exp(k + A\cos\alpha + B\sin\alpha + C\cos 2\alpha + D\sin 2\alpha).$$

Reference: Hendrickson, W. A. & Lattman, E. E. (1970). *Acta Cryst.* B**26**, 136–143.
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.HL_B_iso** (*float*)
The isomorphous Hendrickson–Lattman coefficient $B_{\rm iso}$ for this reflection for this derivative.

$$B_{\rm iso} = -\frac{2.0[F(p)^2_{\rm obs} + F(h)^2_{\rm calc} - F(ph)^2_{\rm obs}]F(p)_{\rm obs}\sin(\alpha_{h\rm calc})}{E^2},$$

where $E = [F(ph)_{\rm obs} - F(p)_{\rm obs} - F(h)_{\rm calc}]^2$ for centric reflections, $E = \{2^{1/2}[F(ph)_{\rm obs} - F(p)_{\rm obs}] - F(h)_{\rm calc}\}^2$ for acentric reflections, $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative, $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model and $\alpha_{h\rm calc}$ = the calculated phase from the heavy-atom model.

This coefficient appears in the expression for the phase probability of each isomorphous derivative:

$$P_i(\alpha) = \exp(k + A\cos\alpha + B\sin\alpha + C\cos 2\alpha + D\sin 2\alpha).$$

Reference: Hendrickson, W. A. & Lattman, E. E. (1970). *Acta Cryst.* B**26**, 136–143.
**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.HL_C_iso** (*float*)
The isomorphous Hendrickson–Lattman coefficient $C_{\rm iso}$ for this reflection for this derivative.

$$C_{\rm iso} = -\frac{F(p)^2_{\rm obs}[\sin(\alpha_{h\rm calc})^2 - \cos(\alpha_{h\rm calc})^2]}{E^2},$$

where $E = [F(ph)_{\rm obs} - F(p)_{\rm obs} - F(h)_{\rm calc}]^2$ for centric reflections, $E = \{2^{1/2}[F(ph)_{\rm obs} - F(p)_{\rm obs}] - F(h)_{\rm calc}\}^2$ for acentric reflections, $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative, $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model and $\alpha_{h\rm calc}$ = the calculated phase from the heavy-atom model.

This coefficient appears in the expression for the phase probability of each isomorphous derivative:

$$P_i(\alpha) = \exp(k + A\cos\alpha + B\sin\alpha + C\cos 2\alpha + D\sin 2\alpha).$$

Reference: Hendrickson, W. A. & Lattman, E. E. (1970). *Acta Cryst.* B**26**, 136–143.

**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.HL_D_iso** (*float*)
The isomorphous Hendrickson–Lattman coefficient $D_{\rm iso}$ for this reflection for this derivative.

$$D_{\rm iso} = -\frac{2.0F(p)^2_{\rm obs}\sin(\alpha_{h\rm calc})^2 + \cos(\alpha_{h\rm calc})^2}{E^2},$$

where $E = [F(ph)_{\rm obs} - F(p)_{\rm obs} - F(h)_{\rm calc}]^2$ for centric reflections, $E = \{2^{1/2}[F(ph)_{\rm obs} - F(p)_{\rm obs}] - F(h)_{\rm calc}\}^2$ for acentric reflections, $F(p)_{\rm obs}$ = the observed structure-factor amplitude of the native, $F(ph)_{\rm obs}$ = the observed structure-factor amplitude of the derivative, $F(h)_{\rm calc}$ = the calculated structure-factor amplitude from the heavy-atom model and $\alpha_{h\rm calc}$ = the calculated phase from the heavy-atom model.

This coefficient appears in the expression for the phase probability of each isomorphous derivative:

$$P_i(\alpha) = \exp(k + A\cos\alpha + B\sin\alpha + C\cos 2\alpha + D\sin 2\alpha).$$

Reference: Hendrickson, W. A. & Lattman, E. E. (1970). *Acta Cryst.* B**26**, 136–143.

**[phasing_MIR_der_refln]**

* **_phasing_MIR_der_refln.index_h** (*int*)
Miller index $h$ for this reflection for this derivative.

**[phasing_MIR_der_refln]**

* **_phasing_MIR_der_refln.index_k** (*int*)
Miller index $k$ for this reflection for this derivative.

**[phasing_MIR_der_refln]**

* **_phasing_MIR_der_refln.index_l** (*int*)
Miller index $l$ for this reflection for this derivative.

**[phasing_MIR_der_refln]**

**_phasing_MIR_der_refln.phase_calc** (*float*)
The calculated value of the structure-factor phase based on the heavy-atom model for this derivative in degrees.

**[phasing_MIR_der_refln]**

* **_phasing_MIR_der_refln.set_id**
This data item is a pointer to **_phasing_set.id** in the PHASING_SET category.

## PHASING_MIR_DER_SHELL

Data items in the PHASING_MIR_DER_SHELL category record statistics, broken down into shells of resolution, for an MIR phasing experiment. This list may contain information from a number of different derivatives; **_phasing_MIR_der_shell.der_id** indicates to which derivative a given record corresponds. (A derivative in this context does not necessarily equate with a data set; see the definition of the PHASING_MIR_DER category for a discussion of the meaning of 'derivative'.)

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR_der_shell.der_id**
**_phasing_MIR_der_shell.d_res_low**
**_phasing_MIR_der_shell.d_res_high**

*Example 1 – based on a paper by Zanotti et al. [J. Biol. Chem. (1993), **268**, 10728–10738] with addition of an arbitrary low-resolution limit.*

```
loop_
_phasing_MIR_der_shell.der_id
_phasing_MIR_der_shell.d_res_low
_phasing_MIR_der_shell.d_res_high
_phasing_MIR_der_shell.ha_ampl
_phasing_MIR_der_shell.loc
 KAu(CN)2  15.0  8.3    54   26
 KAu(CN)2   8.3  6.4    54   20
 KAu(CN)2   6.4  5.2    50   20
 KAu(CN)2   5.2  4.4    44   23
 KAu(CN)2   4.4  3.8    39   23
 KAu(CN)2   3.8  3.4    33   21
 KAu(CN)2   3.4  3.0    28   17
 KAu(CN)2  15.0  3.0    38   21
 K2HgI4    15.0  8.3   149   87
 K2HgI4     8.3  6.4   121   73
 K2HgI4     6.4  5.2    95   61
 K2HgI4     5.2  4.4    80   60
 K2HgI4     4.4  3.8    73   63
 K2HgI4     3.8  3.4    68   57
 K2HgI4     3.4  3.0    63   46
 K2HgI4    15.0  3.0    79   58
 K3IrCl6   15.0  8.3    33   27
 K3IrCl6    8.3  6.4    40   23
 K3IrCl6    6.4  5.2    31   22
 K3IrCl6    5.2  4.4    27   23
 K3IrCl6    4.4  3.8    22   23
 K3IrCl6    3.8  3.4    19   20
 K3IrCl6    3.4  3.0    16   20
 K3IrCl6   15.0  3.0    23   21
```

* **_phasing_MIR_der_shell.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data for this derivative in this shell. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

* **_phasing_MIR_der_shell.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data for this derivative in this shell. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

* **_phasing_MIR_der_shell.der_id**
This data item is a pointer to **_phasing_MIR_der.id** in the PHASING_MIR_DER category.

**_phasing_MIR_der_shell.fom** (*float*)
The mean value of the figure of merit $m$ for reflections in this shell.

$$m = \frac{\int P_\alpha \exp(i\alpha)\,{\rm d}\alpha}{\int P_\alpha\,{\rm d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct; the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.ha_ampl** (*float*)
The mean heavy-atom amplitude for reflections for this derivative in this shell.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.loc** (*float*)
The mean lack-of-closure error loc for reflections for this derivative in this shell.

$$\text{loc} = \sum |F(ph)_{\text{obs}} - F(ph)_{\text{calc}}|,$$

where $F(ph)_{\text{obs}}$ = the observed structure-factor amplitude of the derivative and $F(ph)_{\text{calc}}$ = the calculated structure-factor amplitude of the derivative; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.phase** (*float*)
The mean of the phase values for reflections for this derivative in this shell.
**[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.power** (*float*)
The mean phasing power $P$ for reflections for this derivative in this shell.

$$P = \left( \frac{\sum |F(h)^2_{\text{calc}}|}{\sum |F(ph)_{\text{obs}} - F(ph)_{\text{calc}}|^2} \right)^{1/2},$$

where $F(ph)_{\text{obs}}$ = the observed structure-factor amplitude of this derivative, $F(ph)_{\text{calc}}$ = the calculated structure-factor amplitude of this derivative and $F(h)_{\text{calc}}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.R_cullis** (*float*)
Residual factor $R_{\text{cullis}}$ for centric reflections for this derivative in this shell.

$$R_{\text{cullis}} = \frac{\sum \left| |F(ph)_{\text{obs}} \pm F(p)_{\text{obs}}| - F(h)_{\text{calc}} \right|}{\sum |F(ph)_{\text{obs}} - F(p)_{\text{obs}}|},$$

where $F(p)_{\text{obs}}$ = the observed structure-factor amplitude of the native, $F(ph)_{\text{obs}}$ = the observed structure-factor amplitude of the derivative and $F(h)_{\text{calc}}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.

Reference: Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. London Ser. A*, **265**, 15–38.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.R_kraut** (*float*)
Residual factor $R_{\text{kraut}}$ for general reflections for this derivative in this shell.

$$R_{\text{kraut}} = \frac{\sum |F(ph)_{\text{obs}} - F(ph)_{\text{calc}}|}{\sum |F(ph)_{\text{obs}}|},$$

where $F(ph)_{\text{obs}}$ = the observed structure-factor amplitude of the derivative, $F(ph)_{\text{calc}}$ = the calculated structure-factor amplitude of the derivative and the sum is taken over the specified reflections.

Reference: Kraut, J., Sieker, L. C., High, D. F. & Freer, S. T. (1962). *Proc. Natl Acad. Sci. USA*, **48**, 1417–1424.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_der_shell]**

**_phasing_MIR_der_shell.reflns** (*int*)
The number of reflections in this shell.
The permitted range is $[0, \infty)$. **[phasing_MIR_der_shell]**

## PHASING_MIR_DER_SITE

Data items in the PHASING_MIR_DER_SITE category record details about the heavy-atom sites in an MIR phasing experiment. This list may contain information from a number of different derivatives; **_phasing_MIR_der_site.der_id** indicates to which derivative a given record corresponds. (A derivative in this context does not necessarily equate with a data set; see the definition of the PHASING_MIR_DER category for a discussion of the meaning of 'derivative'.)
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR_der_site.der_id**
**_phasing_MIR_der_site.id**

*Example 1 – based on a paper by Zanotti et al. [J. Biol. Chem. (1993), **268**, 10728–10738] with occupancies converted from electrons to fractional.*

```
loop_
_phasing_MIR_der_site.der_id
_phasing_MIR_der_site.id
_phasing_MIR_der_site.atom_type_symbol
_phasing_MIR_der_site.occupancy
_phasing_MIR_der_site.fract_x
_phasing_MIR_der_site.fract_y
_phasing_MIR_der_site.fract_z
_phasing_MIR_der_site.B_iso
 KAu(CN)2  1  Au  0.40  0.082  0.266  0.615  33.0
 KAu(CN)2  2  Au  0.03  0.607  0.217  0.816  25.9
 KAu(CN)2  3  Au  0.02  0.263  0.782  0.906  15.7
 K2HgI4    1  Hg  0.63  0.048  0.286  0.636  33.7
 K2HgI4    2  Hg  0.34  0.913  0.768  0.889  36.7
 K2HgI4    3  Hg  0.23  0.974  0.455  0.974  24.2
 K2HgI4    4  Hg  0.28  0.903  0.836  0.859  14.7
 K2HgI4    5  Hg  0.07  0.489  0.200  0.885   6.4
 K2HgI4    6  Hg  0.07  0.162  0.799  0.889  32.9
 K3IrCl6   1  Ir  0.26  0.209  0.739  0.758  40.8
 K3IrCl6   2  Ir  0.05  0.279  0.613  0.752  24.9
```

* **_phasing_MIR_der_site.atom_type_symbol**
This data item is a pointer to **_atom_type.symbol** in the ATOM_TYPE category. The scattering factors referenced *via* this data item should be those used in the refinement of the heavy-atom data; in some cases this is the scattering factor for the single heavy atom, in other cases these are the scattering factors for an atomic cluster.

**_phasing_MIR_der_site.B_iso** (*float, su*)
Isotropic displacement parameter for this heavy-atom site in this derivative.
Related item: **_phasing_MIR_der_site.B_iso_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.B_iso_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.B_iso**.
Related item: **_phasing_MIR_der_site.B_iso** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_x** (*float, su*)
The $x$ coordinate of this heavy-atom position in this derivative specified as orthogonal ångströms. The orthogonal Cartesian axes are related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_phasing_MIR_der_site.Cartn_x_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_x_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.Cartn_x**.
Related item: **_phasing_MIR_der_site.Cartn_x** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_y** (*float, su*)
The *y* coordinate of this heavy-atom position in this derivative specified as orthogonal ångströms. The orthogonal Cartesian axes are related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_phasing_MIR_der_site.Cartn_y_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_y_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.Cartn_y**.
Related item: **_phasing_MIR_der_site.Cartn_y** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_z** (*float, su*)
The *z* coordinate of this heavy-atom position in this derivative specified as orthogonal ångströms. The orthogonal Cartesian axes are related to the cell axes as specified by the description given in **_atom_sites.Cartn_transform_axes**.
Related item: **_phasing_MIR_der_site.Cartn_z_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.Cartn_z_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.Cartn_z**.
Related item: **_phasing_MIR_der_site.Cartn_z** (associated value).
**[phasing_MIR_der_site]**

* **_phasing_MIR_der_site.der_id**
This data item is a pointer to **_phasing_MIR_der.id** in the PHASING_MIR_DER category.

**_phasing_MIR_der_site.details** (*text*)
A description of special aspects of the derivative site.
Examples: 'binds to His 117',
'minor site obtained from difference Fourier',
'same as site 2 in the K2HgI4 derivative'.
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_x** (*float, su*)
The *x* coordinate of this heavy-atom position in this derivative specified as a fraction of **_cell.length_a**.
Related item: **_phasing_MIR_der_site.fract_x_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_x_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.fract_x**.
Related item: **_phasing_MIR_der_site.fract_x** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_y** (*float, su*)
The *y* coordinate of this heavy-atom position in this derivative specified as a fraction of **_cell.length_b**.
Related item: **_phasing_MIR_der_site.fract_y_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_y_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.fract_y**.
Related item: **_phasing_MIR_der_site.fract_y** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_z** (*float, su*)
The *z* coordinate of this heavy-atom position in this derivative specified as a fraction of **_cell.length_c**.
Related item: **_phasing_MIR_der_site.fract_z_esd** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.fract_z_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.fract_z**.
Related item: **_phasing_MIR_der_site.fract_z** (associated value).
**[phasing_MIR_der_site]**

* **_phasing_MIR_der_site.id** (*code*)
The value of **_phasing_MIR_der_site.id** must uniquely identify each site in each derivative in the PHASING_MIR_DER_SITE list. The atom identifiers need not be unique over all sites in all derivatives; they need only be unique for each site in each derivative. Note that this item need not be a number; it can be any unique identifier.
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.occupancy** (*float*)
The fraction of the atom type present at this heavy-atom site in a given derivative. The sum of the occupancies of all the atom types at this site may not significantly exceed 1.0 unless it is a dummy site.
The permitted range is $[0.0, \infty)$. Where no value is given, the assumed value is '1.0'.
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.occupancy_anom** (*float, su*)
***_phasing_MIR_der_site.ebi_occupancy_anom*** (*ebi_extensions 1.0*)
The relative anomalous occupancy of the atom type present at this heavy-atom site in a given derivative. This atom occupancy will probably be on an arbitrary scale.
Related item: **_phasing_MIR_der_site.occupancy_anom_su** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.occupancy_anom_su** (*float*)
***_phasing_MIR_der_site.ebi_occupancy_anom_esd*** (*ebi_extensions 1.0*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.occupancy_anom**.
Related item: **_phasing_MIR_der_site.occupancy_anom** (associated value).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.occupancy_iso** (*float, su*)
***_phasing_MIR_der_site.ebi_occupancy_iso*** (*ebi_extensions 1.0*)
The relative real isotropic occupancy of the atom type present at this heavy-atom site in a given derivative. This atom occupancy will probably be on an arbitrary scale.
Related item: **_phasing_MIR_der_site.occupancy_iso_su** (associated esd).
**[phasing_MIR_der_site]**

**_phasing_MIR_der_site.occupancy_iso_su** (*float*)
***_phasing_MIR_der_site.ebi_occupancy_iso_esd*** (*ebi_extensions 1.0*)
The standard uncertainty (estimated standard deviation) of **_phasing_MIR_der_site.occupancy_iso**.
Related item: **_phasing_MIR_der_site.occupancy_iso** (associated value).
**[phasing_MIR_der_site]**

## PHASING_MIR_SHELL

Data items in the PHASING_MIR_SHELL category record statistics for an isomorphous replacement phasing experiment broken down into shells of resolution.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_MIR_shell.d_res_low**
**_phasing_MIR_shell.d_res_high**

*Example 1 – based on a paper by Zanotti et al. [J. Biol. Chem. (1993), **268**, 10728–10738] with addition of an arbitrary low-resolution limit.*

```
loop_
_phasing_MIR_shell.d_res_low
_phasing_MIR_shell.d_res_high
_phasing_MIR_shell.reflns
_phasing_MIR_shell.FOM
 15.0  8.3   80  0.69
  8.3  6.4  184  0.73
  6.4  5.2  288  0.72
  5.2  4.4  406  0.65
  4.4  3.8  554  0.54
  3.8  3.4  730  0.53
  3.4  3.0  939  0.50
```

* **_phasing_MIR_shell.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data in this shell. This is called the highest resolution. Note that the resolution limits of shells in the items **_phasing_MIR_shell.d_res_high** and **_phasing_MIR_shell.d_res_low** are independent of the resolution limits of shells in the items **_reflns_shell.d_res_high** and **_reflns_shell.d_res_low**.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

* **_phasing_MIR_shell.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data in this shell. This is called the lowest resolution. Note that the resolution limits of shells in the items **_phasing_MIR_shell.d_res_high** and **_phasing_MIR_shell.d_res_low** are independent of the resolution limits of shells in the items **_reflns_shell.d_res_high** and **_reflns_shell.d_res_low**.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.FOM** (*float*)
The mean value of the figure of merit $m$ for reflections in this shell.

$$m = \frac{\int P_\alpha \exp(i\alpha)\ \mathrm{d}\alpha}{\int P_\alpha\ \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.FOM_acentric** (*float*)
***_phasing_MIR_shell.ebi_fom_acentric*** (*ebi_extensions 1.0*)
The mean value of the figure of merit $m$ for acentric reflections in this shell.

$$m = \frac{\int P_\alpha \exp(i\alpha)\ \mathrm{d}\alpha}{\int P_\alpha\ \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.FOM_centric** (*float*)
***_phasing_MIR_shell.ebi_fom_centric*** (*ebi_extensions 1.0*)
The mean value of the figure of merit $m$ for centric reflections in this shell.

$$m = \frac{\int P_\alpha \exp(i\alpha)\ \mathrm{d}\alpha}{\int P_\alpha\ \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct and the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.loc** (*float*)
The mean lack-of-closure error loc for reflections in this shell.

$$\mathrm{loc} = \sum |F(ph)_{\mathrm{obs}} - F(ph)_{\mathrm{calc}}|,$$

where $F(ph)_{\mathrm{obs}}$ = the observed structure-factor amplitude of the derivative and $F(ph)_{\mathrm{calc}}$ = the calculated structure-factor amplitude of the derivative; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.mean_phase** (*float*)
The mean of the phase values for all reflections in this shell.
**[phasing_MIR_shell]**

**_phasing_MIR_shell.power** (*float*)
The mean phasing power $P$ for reflections in this shell.

$$P = \left( \frac{\sum |F(h)^2_{\mathrm{calc}}|}{\sum |F(ph)_{\mathrm{obs}} - F(ph)_{\mathrm{calc}}|^2} \right)^{1/2},$$

where $F(ph)_{\mathrm{obs}}$ = the observed structure-factor amplitude of this derivative, $F(ph)_{\mathrm{calc}}$ = the calculated structure-factor amplitude of this derivative and $F(h)_{\mathrm{calc}}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.R_cullis** (*float*)
Residual factor $R_{\mathrm{cullis}}$ for centric reflections in this shell.

$$R_{\mathrm{cullis}} = \frac{\sum \Big| |F(ph)_{\mathrm{obs}} \pm F(p)_{\mathrm{obs}}| - F(h)_{\mathrm{calc}} \Big|}{\sum |F(ph)_{\mathrm{obs}} - F(p)_{\mathrm{obs}}|},$$

where $F(p)_{\mathrm{obs}}$ = the observed structure-factor amplitude of the native, $F(ph)_{\mathrm{obs}}$ = the observed structure-factor amplitude of the derivative and $F(h)_{\mathrm{calc}}$ = the calculated structure-factor amplitude from the heavy-atom model; the sum is taken over the specified reflections.

Reference: Cullis, A. F., Muirhead, H., Perutz, M. F., Rossmann, M. G. & North, A. C. T. (1961). *Proc. R. Soc. London Ser. A*, **265**, 15–38.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.R_kraut** (*float*)
Residual factor $R_{\mathrm{kraut}}$ for general reflections in this shell.

$$R_{\mathrm{kraut}} = \frac{\sum |F(ph)_{\mathrm{obs}} - F(ph)_{\mathrm{calc}}|}{\sum |F(ph)_{\mathrm{obs}}|},$$

where $F(ph)_{\mathrm{obs}}$ = the observed structure-factor amplitude of the derivative and $F(ph)_{\mathrm{calc}}$ = the calculated structure-factor amplitude of the derivative; the sum is taken over the specified reflections.

Reference: Kraut, J., Sieker, L. C., High, D. F. & Freer, S. T. (1962). *Proc. Natl Acad. Sci. USA*, **48**, 1417–1424.
The permitted range is $[0.0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.reflns** (*int*)
The number of reflections in this shell.
The permitted range is $[0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.reflns_acentric** (*int*)
***_phasing_MIR_shell.ebi_reflns_acentric*** (*ebi_extensions 1.0*)
The number of acentric reflections in this shell.
The permitted range is $[0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.reflns_anomalous** (*int*)
The number of anomalous reflections in this shell.
The permitted range is $[0, \infty)$. **[phasing_MIR_shell]**

**_phasing_MIR_shell.reflns_centric** (*int*)
***_phasing_MIR_shell.ebi_reflns_centric*** (*ebi_extensions 1.0*)
The number of centric reflections in this shell.
The permitted range is $[0, \infty)$. **[phasing_MIR_shell]**

## PHASING_SET

Data items in the PHASING_SET category record details about the data sets used in a phasing experiment. A given data set may be used in a number of different ways; for instance, a single data set could be used both as an isomorphous derivative and as a component of a multiple-wavelength calculation. This category establishes identifiers for each data set and permits the archiving of a subset of experimental information for each data set (cell constants, wavelength, temperature *etc.*). This and related categories of data items are provided so that derivative intensity and phase information can be stored in the same data block as the information for the refined structure. If all the possible experimental information for each data set (raw data sets, crystal growth conditions *etc.*) is to be archived, these data items should be recorded in a separate data block.
Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_set.id**

*Example 1 – based on laboratory records for an Hg/Pt derivative of protein NS1.*

```
_phasing_set.id                   'NS1-96'
_phasing_set.cell_angle_alpha     90.0
_phasing_set.cell_angle_beta      90.0
_phasing_set.cell_angle_gamma     90.0
_phasing_set.cell_length_a        38.63
_phasing_set.cell_length_b        38.63
_phasing_set.cell_length_c        82.88
_phasing_set.radiation_wavelength 1.5145
_phasing_set.detector_type        'image plate'
_phasing_set.detector_specific    'RXII'
```

**_phasing_set.cell_angle_alpha** (*float*)
Unit-cell angle $\alpha$ for this data set in degrees.
The permitted range is [0.0, 180.0]. Where no value is given, the assumed value is '90.0'. **[phasing_set]**

**_phasing_set.cell_angle_beta** (*float*)
Unit-cell angle $\beta$ for this data set in degrees.
The permitted range is [0.0, 180.0]. Where no value is given, the assumed value is '90.0'. **[phasing_set]**

**_phasing_set.cell_angle_gamma** (*float*)
Unit-cell angle $\gamma$ for this data set in degrees.
The permitted range is [0.0, 180.0]. Where no value is given, the assumed value is '90.0'. **[phasing_set]**

**_phasing_set.cell_length_a** (*float*)
Unit-cell length *a* for this data set in ångströms.
The permitted range is $[0.0, \infty)$. **[phasing_set]**

**_phasing_set.cell_length_b** (*float*)
Unit-cell length *b* for this data set in ångströms.
The permitted range is $[0.0, \infty)$. **[phasing_set]**

**_phasing_set.cell_length_c** (*float*)
Unit-cell length *c* for this data set in ångströms.
The permitted range is $[0.0, \infty)$. **[phasing_set]**

**_phasing_set.detector_specific** (*text*)
The particular radiation detector. In general, this will be a manufacturer, description, model number or some combination of these.
Examples: 'Siemens model x', 'Kodak XG', 'MAR Research model y'. **[phasing_set]**

**_phasing_set.detector_type** (*text*)
The general class of the radiation detector.
Examples: 'multiwire', 'imaging plate', 'CCD', 'film'. **[phasing_set]**

* **_phasing_set.id** (*line*)
The value of **_phasing_set.id** must uniquely identify a record in the PHASING_SET list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_phasing_set_refln.set_id***,
***_phasing_MAD_set.set_id***,
***_phasing_MIR_der.der_set_id***,
***_phasing_MIR_der.native_set_id***,
***_phasing_MIR_der_refln.set_id***.
Examples: 'KAu(CN)2', 'K2HgI4'. **[phasing_set]**

**_phasing_set.radiation_source_specific** (*text*)
The particular source of radiation. In general, this will be a manufacturer, description, or model number (or some combination of these) for laboratory sources and an institution name and beamline name for synchrotron sources.
Examples: 'Rigaku RU200', 'Philips fine focus Mo', 'NSLS beamline X8C'. **[phasing_set]**

**_phasing_set.radiation_wavelength** (*float*)
The mean wavelength of the radiation used to measure this data set.
The permitted range is $[0.0, \infty)$. **[phasing_set]**

**_phasing_set.temp** (*float*)
The temperature in kelvins at which the data set was measured.
The permitted range is $[0.0, \infty)$. **[phasing_set]**

## PHASING_SET_REFLN

Data items in the PHASING_SET_REFLN category record the values of the measured structure factors used in a phasing experiment. This list may contain information from a number of different data sets; **_phasing_set_refln.set_id** indicates the data set to which a given record corresponds.

Category group(s): **inclusive_group**
**phasing_group**
Category key(s): **_phasing_set_refln.index_h**
**_phasing_set_refln.index_k**
**_phasing_set_refln.index_l**
**_phasing_set_refln.set_id**

*Example 1 – based on laboratory records for the 15,15,32 reflection of an Hg/Pt derivative of protein NS1.*

```
_phasing_set_refln.set_id          'NS1-96'
_phasing_set_refln.index_h          15
_phasing_set_refln.index_k          15
_phasing_set_refln.index_l          32
_phasing_set_refln.F_meas_au       181.79
_phasing_set_refln.F_meas_sigma_au   3.72
```

**_phasing_set_refln.F_meas** (*float, su*)
The measured value of the structure factor for this reflection in this data set in electrons.
Related items: **_phasing_set_refln.F_meas_sigma** (associated esd), **_phasing_set_refln.F_meas_au** (conversion arbitrary).
**[phasing_set_refln]**

**_phasing_set_refln.F_meas_au** (*float, su*)
The measured value of the structure factor for this reflection in this data set in arbitrary units.
Related items: **_phasing_set_refln.F_meas_sigma_au** (associated esd), **_phasing_set_refln.F_meas** (conversion arbitrary). **[phasing_set_refln]**

**_phasing_set_refln.F_meas_sigma** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_set_refln.F_meas** in electrons.
Related items: **_phasing_set_refln.F_meas** (associated value), **_phasing_set_refln.F_meas_sigma_au** (conversion arbitrary).
**[phasing_set_refln]**

**_phasing_set_refln.F_meas_sigma_au** (*float*)
The standard uncertainty (estimated standard deviation) of **_phasing_set_refln.F_meas_au** in arbitrary units.
Related items: **_phasing_set_refln.F_meas_au** (associated value), **_phasing_set_refln.F_meas_sigma** (conversion arbitrary).
**[phasing_set_refln]**

***_phasing_set_refln.index_h** (*int*)
Miller index *h* of this reflection in this data set.
**[phasing_set_refln]**

***_phasing_set_refln.index_k** (*int*)
Miller index *k* of this reflection in this data set.
**[phasing_set_refln]**

***_phasing_set_refln.index_l** (*int*)
Miller index *l* of this reflection in this data set.
**[phasing_set_refln]**

***_phasing_set_refln.set_id**
This data item is a pointer to **_phasing_set.id** in the PHASING_SET category.

## PUBL

Data items in the PUBL category are used when submitting a manuscript for publication.

Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_publ.entry_id**

*Example 1 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C**47**, 2276–2277].*

```
_publ.section_title
;  trans-3-Benzoyl-2-(tert-butyl)-4-(iso-butyl)-
   1,3-oxazolidin-5-one
;

_publ.section_abstract
;  The oxazolidinone ring is a shallow envelope
   conformation with the tert-butyl and iso-butyl groups
   occupying trans-positions with respect to the ring.  The
   angles at the N atom sum to 356.2\%, indicating a very
   small degree of pyramidalization at this atom.  This is
   consistent with electron delocalization between the N
   atom and the carbonyl centre [N-C=O = 1.374(3)\%A].
;
```

*Example 2 – based on $C_{31}H_{48}N_4O_4$, reported by Coleman, Patrick, Andersen & Rettig [Acta Cryst. (1996), C**52**, 1525–1527].*

```
_publ.section_title
;  Hemiasterlin methyl ester
;

_publ.section_title_footnote
;  IUPAC name: methyl 2,5-dimethyl-4-2-[3-methyl-
   2-methylamino-3-(N-methylbenzo[b]pyrrol-
   3-yl)butanamido]-3,3-dimethyl-N-methyl-
   butanamido-2-hexenoate.
;
```

**_publ.contact_author** (*text*)
***_publ_contact_author*** (*cif_core.dic 2.0.1*)
The name and address of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff. It is preferable to use the separate data items **_publ.contact_author_name** and **_publ.contact_author_address**.

Example:
```
; Professor George Ferguson
  Department of Chemistry and Biochemistry
  University of Guelph
  Ontario
  Canada
  N1G 2W1
;
```
**[publ]**

**_publ.contact_author_address** (*text*)
***_publ_contact_author_address*** (*cif_core.dic 2.0.1*)
The address of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff.

Example:
```
; Department of Chemistry and Biochemistry
  University of Guelph
  Ontario
  Canada
  N1G 2W1
;
```
**[publ]**

**_publ.contact_author_email** (*line*)
***_publ_contact_author_email*** (*cif_core.dic 2.0.1*)
E-mail address in a form recognizable to international networks. The format of e-mail addresses is given in Section 3.4, *Address Specification*, of *Internet Message Format*, RFC 2822, P. Resnick (Editor), Network Standards Group, April 2001.
Examples: 'name@host.domain.country', 'uur5@banjo.bitnet'. **[publ]**

**_publ.contact_author_fax** (*line*)
***_publ_contact_author_fax*** (*cif_core.dic 2.0.1*)
Facsimile telephone number of the author submitting the manuscript and data block. The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number with no spaces. The earlier convention of including the international dialing prefix in parentheses is no longer recommended.
Examples: '12(34)9477330', '12()349477330'. **[publ]**

**_publ.contact_author_name** (*text*)
***_publ_contact_author_name*** (*cif_core.dic 2.0.1*)
The name of the author submitting the manuscript and data block. This is the person contacted by the journal editorial staff.
Example:
```
; Professor George Ferguson
;
```
**[publ]**

**_publ.contact_author_phone** (*line*)
***_publ_contact_author_phone*** (*cif_core.dic 2.0.1*)
Telephone number of the author submitting the manuscript and data block. The recommended style starts with the international dialing prefix, followed by the area code in parentheses, followed by the local number and any extension number prefixed by 'x', with no spaces. The earlier convention of including the international dialing prefix in parentheses is no longer recommended.
Examples: '12(34)9477330', '12()349477330', '12(34)9477330x5543'.
**[publ]**

**_publ.contact_letter** (*text*)
***_publ_contact_letter*** (*cif_core.dic 2.0.1*)
A letter submitted to the journal editor by the contact author.
**[publ]**

***_publ.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_publ.manuscript_creation** (*text*)
***_publ_manuscript_creation*** (*cif_core.dic 2.0.1*)
A description of the word-processor package and computer used to create the word-processed manuscript stored as **_publ.manuscript_processed**.
Example: 'Tex file created by FrameMaker on a Sun 3/280'. **[publ]**

**_publ.manuscript_processed** (*text*)
***_publ_manuscript_processed*** (*cif_core.dic 2.0.1*)
The full manuscript of a paper (excluding possibly the figures and the tables) output in ASCII characters from a word processor. Information about the generation of this data item must be specified in the data item **_publ.manuscript_creation**.
**[publ]**

**_publ.manuscript_text** (*text*)
***_publ_manuscript_text*** (*cif_core.dic 2.0.1*)
The full manuscript of a paper (excluding figures and possibly the tables) output as standard ASCII text.
**[publ]**

**_publ.requested_category** (*line*)
***_publ_requested_category*** (*cif_core.dic 2.0.1*)
The category of paper submitted. For submission to *Acta Crystallographica Section C* or *Acta Crystallographica Section E*, *only* the codes indicated for use with these journals should be used.
The data value must be one of the following:

| | |
|---|---|
| FA | Full article |
| FI | Full submission – inorganic (*Acta C*) |
| FO | Full submission – organic (*Acta C*) |
| FM | Full submission – metal-organic (*Acta C*) |
| CI | CIF-access paper – inorganic (*Acta C*) (no longer in use) |
| CO | CIF-access paper – organic (*Acta C*) (no longer in use) |
| CM | CIF-access paper – metal-organic (*Acta C*) (no longer in use) |
| EI | Electronic submission – inorganic (*Acta E*) |
| EO | Electronic submission – organic (*Acta E*) |
| EM | Electronic submission – metal-organic (*Acta E*) |
| AD | Addenda and Errata (*Acta C*, *Acta E*) |
| SC | Short communication |

Where no value is given, the assumed value is 'FA'. **[publ]**

**_publ.requested_coeditor_name** (*line*)
***_publ_requested_coeditor_name*** (*cif_core.dic 2.0.1*)
The name of the co-editor whom the authors would like to handle the submitted manuscript.
**[publ]**

**_publ.requested_journal** (*line*)
***_publ_requested_journal*** (*cif_core.dic 2.0.1*)
The name of the journal to which the manuscript is being submitted.
**[publ]**

**_publ.section_abstract** (*text*)
***_publ_section_abstract*** (*cif_core.dic 2.0.1*)
The abstract section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_acknowledgements** (*text*)
***_publ_section_acknowledgements*** (*cif_core.dic 2.0.1*)
The acknowledgements section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_comment** (*text*)
***_publ_section_comment*** (*cif_core.dic 2.0.1*)
The comment section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_discussion** (*text*)
***_publ_section_discussion*** (*cif_core.dic 2.0.1*)
The discussion section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_experimental** (*text*)
***_publ_section_experimental*** (*cif_core.dic 2.0.1*)
The experimental section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**. The **_publ.section_exptl_prep**, **_publ.section_exptl_solution** and **_publ.section_exptl_refinement** items are preferred for separating the chemical preparation, structure solution and refinement aspects of the description of the experiment.
**[publ]**

**_publ.section_exptl_prep** (*text*)
***_publ_section_exptl_prep*** (*cif_core.dic 2.0.1*)
The experimental preparation section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_exptl_refinement** (*text*)
***_publ_section_exptl_refinement*** (*cif_core.dic 2.0.1*)
The experimental refinement section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_exptl_solution** (*text*)
***_publ_section_exptl_solution*** (*cif_core.dic 2.0.1*)
The experimental solution section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_figure_captions** (*text*)
***_publ_section_figure_captions*** (*cif_core.dic 2.0.1*)
The figure captions section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_introduction** (*text*)
***_publ_section_introduction*** (*cif_core.dic 2.0.1*)
The introduction section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_references** (*text*)
***_publ_section_references*** (*cif_core.dic 2.0.1*)
The references section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_synopsis** (*text*)
***_publ_section_synopsis*** (*cif_core.dic 2.0.1*)
The synopsis section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_table_legends** (*text*)
***_publ_section_table_legends*** (*cif_core.dic 2.0.1*)
The table legends section of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_title** (*text*)
***_publ_section_title*** (*cif_core.dic 2.0.1*)
The title of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

**_publ.section_title_footnote** (*text*)
***_publ_section_title_footnote*** (*cif_core.dic 2.0.1*)
The footnote to the title of a manuscript if the manuscript is submitted in parts. As an alternative see **_publ.manuscript_text** and **_publ.manuscript_processed**.
**[publ]**

## PUBL_AUTHOR

Data items in the PUBL_AUTHOR category record details of the authors of a manuscript submitted for publication.
Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_publ_author.name**

*Example 1 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276–2277].*

```
loop_
_publ_author.name
_publ_author.address
     'Willis, Anthony C.'
;     Research School of Chemistry
      Australian National University
      GPO Box 4
      Canberra, A.C.T.
      Australia    2601
;
```

**_publ_author.address** (*text*)
***_publ_author_address*** (*cif_core.dic 2.0.1*)
The address of a publication author. If there is more than one author this is looped with **_publ_author.name**.
Example:
```
; Department
  Institute
  Street
  City and postcode
  COUNTRY
;
```
**[publ_author]**

**_publ_author.email** (*text*)
***_publ_author_email*** (*cif_core.dic 2.3.1*)
The e-mail address of a publication author. If there is more than one author, this will be looped with **_publ_author.name**. The format of e-mail addresses is given in Section 3.4, *Address Specification*, of *Internet Message Format*, RFC 2822, P. Resnick (Editor), Network Standards Group, April 2001.
Examples: '`name@host.domain.country`', '`bm@iucr.org`'. **[publ_author]**

**_publ_author.footnote** (*line*)
***_publ_author_footnote*** (*cif_core.dic 2.0.1*)
A footnote accompanying an author's name in the list of authors of a paper. Typically indicates sabbatical address, additional affiliations or date of decease.
Examples: '`On leave from U. Western Australia`',
'`Also at Department of Biophysics`'. **[publ_author]**

### _publ_author.id_iucr (*code*)

_publ_author_id_iucr (*cif_core.dic 2.3*)

Identifier in the IUCr contact database of a publication author. This identifier may be available from the *World Directory of Crystallographers* (http://wdc.iucr.org).

Example: '2985'. **[publ_author]**

### *_publ_author.name (*line*)

_publ_author_name (*cif_core.dic 2.0.1*)

The name of a publication author. If there are multiple authors this will be looped with **_publ_author.address**. The family name(s), followed by a comma and including any dynastic components, precedes the first names or initials.

Examples: 'Bleary, Percival R.', 'O'Neil, F.K.', 'Van den Bossche, G.', 'Yang, D.-L.', 'Simonov, Yu.A.'. **[publ_author]**

## PUBL_BODY

Data items in the PUBL_BODY category permit the labelling of different text sections within the body of a paper. Note that these should not be used in a paper which has a standard format with sections tagged by specific data names (such as in *Acta Crystallographica Section C*). Typically, each journal will supply a list of the specific items it requires in its *Notes for Authors*.

Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_publ_body.element**
**_publ_body.label**

*Example 1 – based on a paper by R. Restori & D. Schwarzenbach [Acta Cryst. (1996), A52, 369–378].*

```
loop_
_publ_body.element
_publ_body.label
_publ_body.title
_publ_body.format
_publ_body.contents

     section   1         Introduction                    cif
; X-ray diffraction from a crystalline material provides
  information on the thermally and spatially averaged
  electron density in the crystal...
;
     section   2         Theory                         tex
; In the rigid-atom approximation, the dynamic electron
  density of an atom is described by the convolution
  product of the static atomic density and a probability
  density function,
  $\rho_dyn(\bf r) = \rho_stat(\bf r) * P(\bf r). \eqno(1)$
;
```

*Example 2 – based on a paper by R. J. Papoular, Y. Vekhter & P. Coppens [Acta Cryst. (1996), A52, 397–407].*

```
loop_
_publ_body.element
_publ_body.label
_publ_body.title
_publ_body.contents

     section     3
; The two-channel method for retrieval of the deformation
  electron density
;
     .
     subsection  3.1  'The two-channel entropy S[\D\r(r)]'
; As the wide dynamic range involved in the total electron
  density...
;
     subsection  3.2
'Uniform vs informative prior model densities'        .
     subsubsection  3.2.1  'Use of uniform models'
; Straightforward algebra leads to expressions analogous
  to...
;
```

### _publ_body.contents (*text*)

_publ_body_contents (*cif_core.dic 2.0.1*)

A text section of a paper.

**[publ_body]**

### _publ_body.element (*code*)

_publ_body_element (*cif_core.dic 2.0.1*)

The functional role of the associated text section.

The data value must be one of the following:

- section
- subsection
- subsubsection
- appendix
- footnote

**[publ_body]**

### _publ_body.format (*code*)

_publ_body_format (*cif_core.dic 2.0.1*)

Code indicating the appropriate typesetting conventions for accented characters and special symbols in the text section.

The data value must be one of the following:

| | |
|---|---|
| ascii | no coding for special symbols |
| cif | CIF convention |
| latex | LaTeX |
| sgml | SGML (ISO 8879) |
| tex | TeX |
| troff | troff or nroff |

**[publ_body]**

### _publ_body.label (*code*)

_publ_body_label (*cif_core.dic 2.0.1*)

Code identifying the section of text.

Examples: '1', '1.1', '2.1.3'. **[publ_body]**

### _publ_body.title (*text*)

_publ_body_title (*cif_core.dic 2.0.1*)

Title of the associated section of text.

**[publ_body]**

## PUBL_MANUSCRIPT_INCL

Data items in the PUBL_MANUSCRIPT_INCL category allow the authors of a manuscript submitted for publication to list data names that should be added to the standard request list used by the journal printing software.

Category group(s): **inclusive_group**
**iucr_group**
Category key(s): **_publ_manuscript_incl.entry_id**

*Example 1 – hypothetical example.*

```
_publ_manuscript_incl.entry_id   'EXAMHYPO'
loop_
_publ_manuscript_incl.extra_item
_publ_manuscript_incl.extra_info
_publ_manuscript_incl.extra_defn
'_atom_site.symmetry_multiplicity'
     'to emphasise special sites'  yes
'_chemical.compound_source'
     'rare material, unusual source'   yes
'_reflns.d_resolution_high'
     'limited data are a problem here'  yes
'_crystal.magnetic_permeability'
     'unusual value for this material'  no
```

### *_publ_manuscript_incl.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### _publ_manuscript_incl.extra_defn (*line*)

*_publ_manuscript_incl_extra_defn* (*cif_core.dic 2.0.1*)

Flags whether the corresponding data item marked for inclusion in a journal request list is a standard CIF definition or not.

The data value must be one of the following:

| | |
|---|---|
| no | not a standard CIF data name |
| n | abbreviation for 'no' |
| yes | a standard CIF data name |
| y | abbreviation for 'yes' |

**[publ_manuscript_incl]**

### _publ_manuscript_incl.extra_info (*text*)

*_publ_manuscript_incl_extra_info* (*cif_core.dic 2.0.1*)

A short note indicating the reason why the author wishes the corresponding data item marked for inclusion in the journal request list to be published.

Examples: 'to emphasise very special sites',
'rare material from unusual source',
'the limited data is a problem here',
'a new data quantity needed here'. **[publ_manuscript_incl]**

### _publ_manuscript_incl.extra_item (*line*)

*_publ_manuscript_incl_extra_item* (*cif_core.dic 2.0.1*)

Specifies the inclusion of specific data into a manuscript which are not normally requested by the journal. The values of this item are the extra data names (which *must* be enclosed in single quotes) that will be added to the journal request list.

Examples: '_atom_site.symmetry_multiplicity',
'_chemical.compound_source', '_reflns.d_resolution_high',
'_crystal.magnetic_permeability'. **[publ_manuscript_incl]**

## REFINE

Data items in the REFINE category record details about the structure-refinement parameters.

Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_refine.entry_id                          '5HVP'
_refine.ls_number_reflns_obs              12901
_refine.ls_number_restraints              6609
_refine.ls_number_parameters              7032
_refine.ls_R_Factor_obs                   0.176
_refine.ls_weighting_scheme               calc
_refine.ls_weighting_details
; Sigdel model of Konnert-Hendrickson:
  Sigdel: Afsig +  Bfsig*(sin(theta)/lambda-1/6)
  Afsig = 22.0, Bfsig = -150.0 at beginning of refinement
  Afsig = 15.5, Bfsig =  -50.0 at end of refinement
;
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C47, 2276–2277].*

```
_refine.details             sfls:_F_calc_weight_full_matrix

_refine.ls_structure_factor_coef  F
_refine.ls_matrix_type            full
_refine.ls_weighting_scheme       calc
_refine.ls_weighting_details     'w=1/(\s^2^(F)+0.0004F^2^)'
_refine.ls_hydrogen_treatment    'refxyz except H332B noref'
_refine.ls_extinction_method      Zachariasen
_refine.ls_extinction_coef        3514
_refine.ls_extinction_expression
; Larson, A. C. (1970). "Crystallographic Computing", edited
  by F. R. Ahmed. Eq. (22) p. 292. Copenhagen: Munksgaard.

_refine.ls_abs_structure_details
; The absolute configuration was assigned to agree with the
  known chirality at C3 arising from its precursor l-leucine.
;
_refine.ls_abs_structure_Flack      0
_refine.ls_number_reflns_obs     1408
_refine.ls_number_parameters      272
_refine.ls_number_restraints        0
_refine.ls_number_constraints       0
_refine.ls_R_factor_all              .038
_refine.ls_R_factor_obs              .034
_refine.ls_wR_factor_all             .044
_refine.ls_wR_factor_obs             .042
_refine.ls_goodness_of_fit_all      1.462
_refine.ls_goodness_of_fit_obs      1.515
_refine.ls_shift_over_esd_max        .535
_refine.ls_shift_over_esd_mean       .044
_refine.diff_density_min            -.108
_refine.diff_density_max             .131
```

### _refine.aniso_B[1][1] (*float*)

The [1][1] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.aniso_B[1][2] (*float*)

The [1][2] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.aniso_B[1][3] (*float*)

The [1][3] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.aniso_B[2][2] (*float*)

The [2][2] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.aniso_B[2][3] (*float*)

The [2][3] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.aniso_B[3][3] (*float*)

The [3][3] element of the matrix that defines the overall anisotropic displacement model if one was refined for this structure.

**[refine]**

### _refine.B_iso_max (*float*)

The maximum isotropic displacement parameter ($B$ value) found in the coordinate set.

**[refine]**

**_refine.B_iso_mean** (*float*)
The mean isotropic displacement parameter ($B$ value) for the coordinate set.
**[refine]**

**_refine.B_iso_min** (*float*)
The minimum isotropic displacement parameter ($B$ value) found in the coordinate set.
**[refine]**

**_refine.correlation_coeff_Fo_to_Fc** (*float*)
***_refine.ebi_Correlation_coeff_Fo_to_Fc*** (*ebi_extensions 1.0*)
The correlation coefficient between the observed and calculated structure factors for reflections included in the refinement. The correlation coefficient is scale-independent and gives an idea of the quality of the refined model.

$$R_{\rm corr} = \frac{\sum_i (F_{oi}F_{ci} - \langle F_o\rangle\langle F_c\rangle)}{\sqrt{\sum_i (F_{oi})^2 - \langle F_o\rangle^2}\sqrt{\sum_i (F_{ci})^2 - \langle F_c\rangle^2}},$$

where $F_o$ = observed structure factors, $F_c$ = calculated structure factors, $\langle\rangle$ denotes average value and the summation is over reflections included in the refinement.
**[refine]**

**_refine.correlation_coeff_Fo_to_Fc_free** (*float*)
***_refine.ebi_Correlation_coeff_Fo_to_Fc_free*** (*ebi_extensions 1.0*)
The correlation coefficient between the observed and calculated structure factors for reflections not included in the refinement (free reflections). The correlation coefficient is scale-independent and gives an idea of the quality of the refined model.

$$R_{\rm corr} = \frac{\sum_i (F_{oi}F_{ci} - \langle F_o\rangle\langle F_c\rangle)}{\sqrt{\sum_i (F_{oi})^2 - \langle F_o\rangle^2}\sqrt{\sum_i (F_{ci})^2 - \langle F_c\rangle^2}},$$

where $F_o$ = observed structure factors, $F_c$ = calculated structure factors, $\langle\rangle$ denotes average value and the summation is over reflections not included in the refinement (free reflections).
**[refine]**

**_refine.details** (*text*)
***_refine_special_details*** (*cif_core.dic 2.0.1*)
Description of special aspects of the refinement process.
**[refine]**

**_refine.diff_density_max** (*float, su*)
***_refine_diff_density_max*** (*cif_core.dic 2.0.1*)
The maximum value of the electron density in the final difference Fourier map.
Related item: **_refine.diff_density_max_esd** (associated esd). **[refine]**

**_refine.diff_density_max_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.diff_density_max**.
Related item: **_refine.diff_density_max** (associated value). **[refine]**

**_refine.diff_density_min** (*float, su*)
***_refine_diff_density_min*** (*cif_core.dic 2.0.1*)
The minimum value of the electron density in the final difference Fourier map.
Related item: **_refine.diff_density_min_esd** (associated esd). **[refine]**

**_refine.diff_density_min_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.diff_density_min**.
Related item: **_refine.diff_density_min** (associated value). **[refine]**

**_refine.diff_density_rms** (*float, su*)
***_refine_diff_density_rms*** (*cif_core.dic 2.0.1*)
The root-mean-square-deviation of the electron density in the final difference Fourier map. This value is measured with respect to the arithmetic mean density and is derived from summations over each grid point in the asymmetric unit of the cell. This quantity is useful for assessing the significance of the values of **_refine.diff_density_min** and **_refine.diff_density_max**, and also for defining suitable contour levels.
Related item: **_refine.diff_density_rms_esd** (associated esd). **[refine]**

**_refine.diff_density_rms_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.diff_density_rms**.
Related item: **_refine.diff_density_rms** (associated value). **[refine]**

***_refine.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_refine.ls_abs_structure_details** (*text*)
***_refine_ls_abs_structure_details*** (*cif_core.dic 2.0.1*)
The nature of the absolute structure and how it was determined. For example, this may describe the Friedel pairs used.
**[refine]**

**_refine.ls_abs_structure_Flack** (*float, su*)
***_refine_ls_abs_structure_Flack*** (*cif_core.dic 2.0.1*)
The measure of absolute structure (enantiomorph or polarity) as defined by Flack (1983). For centrosymmetric structures the only permitted value, if the data name is present, is 'inapplicable', represented by '.' . For noncentrosymmetric structures the value must lie in the 99.97% Gaussian confidence interval $-3u \le x \le 1+3u$ and a standard uncertainty (estimated standard deviation) $u$ must be supplied. The item range of $[0.0, 1.0]$ is correctly interpreted as meaning $(0.0-3u) \le x \le (1.0+3u)$.

Reference: Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

The permitted range is [0.0, 1.0].
Related item: **_refine.ls_abs_structure_Flack_esd** (associated esd).
**[refine]**

**_refine.ls_abs_structure_Flack_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.ls_abs_structure_Flack**.
Related item: **_refine.ls_abs_structure_Flack** (associated value). **[refine]**

**_refine.ls_abs_structure_Rogers** (*float, su*)
***_refine_ls_abs_structure_Rogers*** (*cif_core.dic 2.0.1*)
The measure of absolute structure (enantiomorph or polarity) as defined by Rogers. The value must lie in the 99.97% Gaussian confidence interval $-1-3u \le \eta \le 1+3u$ and a standard uncertainty (estimated standard deviation) $u$ must be supplied. The item range of $[-1.0, 1.0]$ is correctly interpreted as meaning $(-1.0-3u) \le \eta \le (1.0+3u)$.

Reference: Rogers, D. (1981). *Acta Cryst.* A**37**, 734–741.

The permitted range is [−1.0, 1.0].
Related item: **_refine.ls_abs_structure_Rogers_esd** (associated esd).
**[refine]**

**_refine.ls_abs_structure_Rogers_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.ls_abs_structure_Rogers**.
Related item: **_refine.ls_abs_structure_Rogers** (associated value). **[refine]**

***_refine.ls_d_res_high** (*float*)
***_refine_ls_d_res_high*** (*cif_core.dic 2.0.1*)
The smallest value for the interplanar spacings for the reflection data used in the refinement in ångströms. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[refine]**

***_refine.ls_d_res_low** (*float*)
***_refine_ls_d_res_low*** (*cif_core.dic 2.0.1*)
The largest value for the interplanar spacings for the reflection data used in the refinement in ångströms. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_extinction_coef** (*float, su*)
***_refine_ls_extinction_coef*** (*cif_core.dic 2.0.1*)
The extinction coefficient used to calculate the correction factor applied to the structure-factor data. The nature of the extinction coefficient is given in the definitions of **_refine.ls_extinction_expression** and **_refine.ls_extinction_method**. For the 'Zachariasen' method it is the $r^*$ value; for the 'Becker–Coppens type 1 isotropic' method it is the '$g$' value, and for 'Becker–Coppens type 2 isotropic' corrections it is the '$\rho$' value. Note that the magnitude of these values is usually of the order of 10 000.

References: Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–147, 148–153. Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564. Larson, A. C. (1967). *Acta Cryst.* **23**, 664–665.
Related item: **_refine.ls_extinction_coef_esd** (associated esd) .
Example: '3472' (Zachariasen coefficient r* = 0.347 E04). **[refine]**

**_refine.ls_extinction_coef_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.ls_extinction_coef**.
Related item: **_refine.ls_extinction_coef** (associated value). **[refine]**

**_refine.ls_extinction_expression** (*text*)
***_refine_ls_extinction_expression*** (*cif_core.dic 2.0.1*)
A description of or reference to the extinction-correction equation used to apply the data item **_refine.ls_extinction_coef**. This information must be sufficient to reproduce the extinction-correction factors applied to the structure factors.
Example:
```
; Larson, A. C. (1970). "Crystallographic Computing", edited
by  F. R. Ahmed. Eq. (22), p.292. Copenhagen: Munksgaard.
;
```
**[refine]**

**_refine.ls_extinction_method** (*text*)
***_refine_ls_extinction_method*** (*cif_core.dic 2.0.1*)
A description of the extinction-correction method applied. This description should include information about the correction method, either 'Becker–Coppens' or 'Zachariasen'. The latter is sometimes referred to as the 'Larson' method even though it employs Zachariasen's formula. The Becker–Coppens procedure is referred to as 'type 1' when correcting secondary extinction dominated by the mosaic spread; as 'type 2' when secondary extinction is dominated by particle size and includes a primary extinction component; and as 'mixed' when there is a mixture of types 1 and 2. For the Becker–Coppens method, it is also necessary to set the mosaic distribution as either 'Gaussian' or 'Lorentzian' and the nature of the extinction as 'isotropic' or 'anisotropic'. Note that if either the 'mixed' or 'anisotropic' corrections are applied the multiple coefficients cannot be contained in ***_extinction_coef** and must be listed in **_refine.details**.

References: Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* A**30**, 129–147, 148–153. Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564. Larson, A. C. (1967). *Acta Cryst.* **23**, 664–665.
Example: 'B-C type 2 Gaussian isotropic'. **[refine]**

**_refine.ls_goodness_of_fit_all** (*float, su*)
***_refine_ls_goodness_of_fit_all*** (*cif_core.dic 2.0.1*)
The least-squares goodness-of-fit parameter $S$ for all data after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also the definition of **_refine.ls_restrained_S_all**.

$$S = \left( \frac{\sum \left| w \left| Y_{\rm obs} - Y_{\rm calc} \right|^2 \right|}{N_{\rm ref} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight [1/(e.s.d. squared)], $N_{\rm ref}$ = the number of reflections used in the refinement and $N_{\rm param}$ = the number of refined parameters; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_goodness_of_fit_all_esd** (associated esd).
**[refine]**

**_refine.ls_goodness_of_fit_all_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.ls_goodness_of_fit_all**.
Related item: **_refine.ls_goodness_of_fit_all** (associated value). **[refine]**

**_refine.ls_goodness_of_fit_gt** (*float*)
***_refine_ls_goodness_of_fit_gt*** (*cif_core.dic 2.3*)
The least-squares goodness-of-fit parameter $S$ for significantly intense reflections (see **_reflns.threshold_expression**) after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also **_refine.ls_restrained_S_** definitions.

$$S = \left( \frac{\sum \left| w \left| Y_{\rm obs} - Y_{\rm calc} \right|^2 \right|}{N_{\rm ref} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight $[1/(u^2)]$, $u$ = the standard uncertainty, $N_{\rm ref}$ = the number of reflections used in the refinement and $N_{\rm param}$ = the number of refined parameters; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_goodness_of_fit_obs** (alternate). **[refine]**

**_refine.ls_goodness_of_fit_obs** (*float, su*)
***_refine_ls_goodness_of_fit_obs*** (*cif_core.dic 2.0.1*)
The least-squares goodness-of-fit parameter $S$ for reflection data classified as 'observed' (see **_reflns.observed_criterion**) after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also the definition of **_refine.ls_restrained_S_obs**.

$$S = \left( \frac{\sum |w|Y_{\rm obs} - Y_{\rm calc}|^2|}{N_{\rm ref} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight [1/(e.s.d. squared)], $N_{\rm ref}$ = the number of reflections used in the refinement and $N_{\rm param}$ = the number of refined parameters; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_goodness_of_fit_obs_esd** (associated esd).
**[refine]**

**_refine.ls_goodness_of_fit_obs_esd** (*float*)
The standard uncertainty (estimated standard deviation) of **_refine.ls_goodness_of_fit_obs**.
Related item: **_refine.ls_goodness_of_fit_obs** (associated value). **[refine]**

**_refine.ls_goodness_of_fit_ref** (*float*)
***_refine_ls_goodness_of_fit_ref*** (*cif_core.dic 2.3*)
The least-squares goodness-of-fit parameter $S$ for all reflections included in the refinement after the final cycle of refinement. Ideally, account should be taken of parameters restrained in the least-squares refinement. See also **_refine.ls_restrained_S_** definitions.

$$S = \left( \frac{\sum |w|Y_{\rm obs} - Y_{\rm calc}|^2|}{N_{\rm ref} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight $[1/(u^2)]$, $u$ = the standard uncertainty, $N_{\rm ref}$ = the number of reflections used in the refinement and $N_{\rm param}$ = the number of refined parameters; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_hydrogen_treatment** (*ucode*)
***_refine_ls_hydrogen_treatment*** (*cif_core.dic 2.0.1*)
Treatment of hydrogen atoms in the least-squares refinement.
The data value must be one of the following:

| | |
|---|---|
| `refall` | refined all H-atom parameters |
| `refxyz` | refined H-atom coordinates only |
| `refU` | refined H-atom $U$'s only |
| `noref` | no refinement of H-atom parameters |
| `constr` | H-atom parameters constrained |
| `mixed` | some constrained, some independent |
| `undef` | H-atom parameters not defined |

**[refine]**

**_refine.ls_matrix_type** (*ucode*)
***_refine_ls_matrix_type*** (*cif_core.dic 2.0.1*)
Type of matrix used to accumulate the least-squares derivatives.
The data value must be one of the following:

| | |
|---|---|
| `full` | full |
| `fullcycle` | full with fixed elements per cycle |
| `atomblock` | block diagonal per atom |
| `userblock` | user-defined blocks |
| `diagonal` | diagonal elements only |
| `sparse` | selected elements only |

**[refine]**

**_refine.ls_number_constraints** (*int*)
***_refine_ls_number_constraints*** (*cif_core.dic 2.0.1*)
The number of constrained (non-refined or dependent) parameters in the least-squares process. These may be due to symmetry or any other constraint process (*e.g.* rigid-body refinement). See also **_atom_site.constraints** and **_atom_site.refinement_flags**. A general description of constraints may appear in **_refine.details**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_parameters** (*int*)
***_refine_ls_number_parameters*** (*cif_core.dic 2.0.1*)
The number of parameters refined in the least-squares process. If possible, this number should include some contribution from the restrained parameters. The restrained parameters are distinct from the constrained parameters (where one or more parameters are linearly dependent on the refined value of another). Least-squares restraints often depend on geometry or energy considerations and this makes their direct contribution to this number, and to the goodness-of-fit calculation, difficult to assess.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_reflns_all** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_reflns_obs** (*int*)
***_refine_ls_number_reflns*** (*cif_core.dic 2.0.1*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_reflns_R_free** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_reflns_R_work** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_number_restraints** (*int*)
***_refine_ls_number_restraints*** (*cif_core.dic 2.0.1*)
The number of restrained parameters. These are parameters which are not directly dependent on another refined parameter. Restrained parameters often involve geometry or energy dependencies. See also **_atom_site.constraints** and **_atom_site.refinement_flags**. A general description of refinement constraints may appear in **_refine.details**.
The permitted range is $[0, \infty)$. **[refine]**

**_refine.ls_percent_reflns_obs** (*float*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, expressed as a percentage of the number of geometrically observable reflections that satisfy the resolution limits.
**[refine]**

**_refine.ls_percent_reflns_R_free** (*float*)
The number of reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' *R* factor, expressed as a percentage of the number of geometrically observable reflections that satisfy the resolution limits.
**[refine]**

**_refine.ls_R_factor_all** (*float*)
***_refine_ls_R_factor_all*** (*cif_core.dic 2.0.1*)
Residual factor *R* for all reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_wR_factor_all** (alternate). **[refine]**

**_refine.ls_R_factor_gt** (*float*)
***_refine_ls_R_factor_gt*** (*cif_core.dic 2.3*)
Residual factor for the reflections (with number given by **_reflns.number_gt**) judged significantly intense (*i.e.* satisfying the threshold specified by **_reflns.threshold_expression**) and included in the refinement. The reflections also satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low**. This is the conventional *R* factor. See also **_refine.ls_wR_factor_** definitions.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_R_factor_obs** (alternate). **[refine]**

**_refine.ls_R_factor_obs** (*float*)
***_refine_ls_R_factor_obs*** (*cif_core.dic 2.0.1*)
Residual factor *R* for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**. **_refine.ls_R_factor_obs** should not be confused with **_refine.ls_R_factor_R_work**; the former reports the results of a refinement in which all observed reflections were used, the latter a refinement in which a subset of the observed reflections were excluded from refinement for the calculation of a 'free' *R* factor. However, it would be meaningful to quote both values if a 'free' *R* factor were calculated for most of the refinement, but all of the observed reflections were used in the final rounds of refinement; such a protocol should be explained in **_refine.details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_wR_factor_obs** (alternate). **[refine]**

**_refine.ls_R_factor_R_free** (*float*)
Residual factor *R* for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' *R* factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related items: **_refine.ls_wR_factor_R_free** (alternate), **_refine.ls_R_factor_R_free_error** (associated error). **[refine]**

**_refine.ls_R_factor_R_free_error** (*float*)
The estimated error in **_refine.ls_R_factor_R_free**. The method used to estimate the error is described in the item **_refine.ls_R_factor_R_free_error_details**.
Related item: **_refine.ls_R_factor_R_free** (associated value). **[refine]**

**_refine.ls_R_factor_R_free_error_details** (*text*)
Special aspects of the method used to estimate the error in **_refine.ls_R_factor_R_free**.
**[refine]**

**_refine.ls_R_factor_R_work** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**. **_refine.ls_R_factor_obs** should not be confused with **_refine.ls_R_factor_R_work**; the former reports the results of a refinement in which all observed reflections were used, the latter a refinement in which a subset of the observed reflections were excluded from refinement for the calculation of a 'free' $R$ factor. However, it would be meaningful to quote both values if a 'free' $R$ factor were calculated for most of the refinement, but all of the observed reflections were used in the final rounds of refinement; such a protocol should be explained in **_refine.details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine.ls_wR_factor_R_work** (alternate). **[refine]**

**_refine.ls_R_Fsqd_factor_obs** (*float*)
***_refine_ls_R_Fsqd_factor*** (*cif_core.dic 2.0.1*)
Residual factor $R(F^2)$ for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, calculated on the squares of the observed and calculated structure-factor amplitudes.

$$R(F^2) = \frac{\sum |F^2_{\rm obs} - F^2_{\rm calc}|}{\sum |F^2_{\rm obs}|},$$

where $F^2_{\rm obs}$ = squares of the observed structure-factor amplitudes, $F^2_{\rm calc}$ = squares of the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_R_I_factor_obs** (*float*)
***_refine_ls_R_I_factor*** (*cif_core.dic 2.0.1*)
Residual factor $R(I)$ for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, calculated on the estimated reflection intensities. This is most often calculated in Rietveld refinements against powder data, where it is referred to as $R_B$ or $R_{\rm Bragg}$.

$$R(I) = \frac{\sum |I_{\rm obs} - I_{\rm calc}|}{\sum |I_{\rm obs}|},$$

where $I_{\rm obs}$ = the net observed intensities, $I_{\rm calc}$ = the net calculated intensities and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_redundancy_reflns_all** (*float*)
The ratio of the total number of observations of the reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** to the number of crystallographically unique reflections that satisfy the same limits.
**[refine]**

**_refine.ls_redundancy_reflns_obs** (*float*)
The ratio of the total number of observations of the reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion** to the number of crystallographically unique reflections that satisfy the same limits.
**[refine]**

**_refine.ls_restrained_S_all** (*float*)
***_refine_ls_restrained_S_all*** (*cif_core.dic 2.0.1*)
The least-squares goodness-of-fit parameter $S'$ for all reflections after the final cycle of least-squares refinement. This parameter explicitly includes the restraints applied in the least-squares process. See also the definition of **_refine.ls_goodness_of_fit_all**.

$$S' = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right| + \sum_r \left| w_r |P_{\rm calc} - P_{\rm targ}|^2 \right|}{N_{\rm ref} + N_{\rm restr} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight [1/(e.s.d. squared)], $P_{\rm calc}$ = the calculated restraint values, $P_{\rm targ}$ = the target restraint values, $w_r$ = the restraint weight, $N_{\rm ref}$ = the number of reflections used in the refinement (see **_refine.ls_number_reflns_obs**), $N_{\rm restr}$ = the number of restraints (see **_refine.ls_number_restraints**) and $N_{\rm param}$ = the number of refined parameters (see **_refine.ls_number_parameters**); the sum $\sum$ is taken over the specified reflections and the sum $\sum_r$ is taken over the restraints.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_restrained_S_obs** (*float*)
***_refine_ls_restrained_S_obs*** (*cif_core.dic 2.0.1*)
The least-squares goodness-of-fit parameter $S'$ for reflection data classified as observed (see **_reflns.observed_criterion**) after the final cycle of least-squares refinement. This parameter explicitly includes the restraints applied in the least-squares process. See also the definition of **_refine.ls_goodness_of_fit_obs**.

$$S' = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right| + \sum_r \left| w_r |P_{\rm calc} - P_{\rm targ}|^2 \right|}{N_{\rm ref} + N_{\rm restr} - N_{\rm param}} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed coefficients (see **_refine.ls_structure_factor_coef**), $Y_{\rm calc}$ = the calculated coefficients (see **_refine.ls_structure_factor_coef**), $w$ = the least-squares reflection weight [1/(e.s.d. squared)], $P_{\rm calc}$ = the calculated restraint values, $P_{\rm targ}$ = the target restraint values, $w_r$ = the restraint weight, $N_{\rm ref}$ = the number of reflections used in the refinement (see **_refine.ls_number_reflns_obs**), $N_{\rm restr}$ = the number of restraints (see **_refine.ls_number_restraints**) and $N_{\rm param}$ = the number of refined parameters (see **_refine.ls_number_parameters**); the sum $\sum$ is taken over the specified reflections and the sum $\sum_r$ is taken over the restraints.
The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.ls_shift_over_esd_max** (*float*)
***_refine_ls_shift/esd_max*** (*cif_core.dic 2.0.1*)
The largest ratio of the final least-squares parameter shift to the final standard uncertainty (estimated standard deviation).
The permitted range is $[0.0, \infty)$. **[refine]**

### _refine.ls_shift_over_esd_mean (*float*)

***_refine_ls_shift/esd_mean*** (*cif_core.dic 2.0.1*)

The average ratio of the final least-squares parameter shift to the final standard uncertainty (estimated standard deviation).

The permitted range is $[0.0, \infty)$. **[refine]**

### _refine.ls_shift_over_su_max (*float*)

***_refine_ls_shift/su_max*** (*cif_core.dic 2.3*)

The largest ratio of the final least-squares parameter shift to the final standard uncertainty.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_shift_over_esd_max** (alternate). **[refine]**

### _refine.ls_shift_over_su_max_lt (*float*)

***_refine_ls_shift/su_max_lt*** (*cif_core.dic 2.3*)

An upper limit for the largest ratio of the final least-squares parameter shift to the final standard uncertainty. This item is used when the largest value of the shift divided by the final standard uncertainty is too small to measure.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_shift_over_su_max** (alternate). **[refine]**

### _refine.ls_shift_over_su_mean (*float*)

***_refine_ls_shift/su_mean*** (*cif_core.dic 2.3*)

The average ratio of the final least-squares parameter shift to the final standard uncertainty.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_shift_over_esd_mean** (alternate). **[refine]**

### _refine.ls_shift_over_su_mean_lt (*float*)

***_refine_ls_shift/su_mean_lt*** (*cif_core.dic 2.3*)

An upper limit for the average ratio of the final least-squares parameter shift to the final standard uncertainty. This item is used when the average value of the shift divided by the final standard uncertainty is too small to measure.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_shift_over_su_mean** (alternate). **[refine]**

### _refine.ls_structure_factor_coef (*ucode*)

***_refine_ls_structure_factor_coef*** (*cif_core.dic 2.0.1*)

Structure-factor coefficient $|F|$, $F^2$ or $I$ used in the least-squares refinement process.

The data value must be one of the following:

| | |
|---|---|
| F | structure-factor magnitude |
| Fsqd | structure factor squared |
| Inet | net intensity |

**[refine]**

### _refine.ls_weighting_details (*text*)

***_refine_ls_weighting_details*** (*cif_core.dic 2.0.1*)

A description of special aspects of the weighting scheme used in least-squares refinement. Used to describe the weighting when the value of **_refine.ls_weighting_scheme** is specified as 'calc'.

Example:

```
; Sigdel model of Konnert-Hendrickson:
  Sigdel =
  Afsig +  Bfsig*(sin(theta)/lambda-1/6)
  Afsig = 22.0, Bfsig = 150.0
  at the beginning of refinement.
  Afsig = 16.0, Bfsig =  60.0
  at the end of refinement.
;
```

**[refine]**

### _refine.ls_weighting_scheme (*ucode*)

***_refine_ls_weighting_scheme*** (*cif_core.dic 2.0.1*)

The weighting scheme applied in the least-squares process. The standard code may be followed by a description of the weight (but see **_refine.ls_weighting_details** for a preferred approach).

The data value must be one of the following:

| | |
|---|---|
| sigma | based on measured e.s.d.'s |
| unit | unit or no weights applied |
| calc | calculated weights applied |

**[refine]**

### _refine.ls_wR_factor_all (*float*)

***_refine_ls_wR_factor_all*** (*cif_core.dic 2.0.1*)

Weighted residual factor $wR$ for all reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_R_factor_all** (alternate). **[refine]**

### _refine.ls_wR_factor_obs (*float*)

***_refine_ls_wR_factor_obs*** (*cif_core.dic 2.0.1*)

Weighted residual factor $wR$ for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_R_factor_obs** (alternate). **[refine]**

### _refine.ls_wR_factor_R_free (*float*)

Weighted residual factor $wR$ for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_R_factor_R_free** (alternate). **[refine]**

**_refine.ls_wR_factor_R_work** (*float*)

Weighted residual factor *wR* for reflections that satisfy the resolution limits established by **_refine.ls_d_res_high** and **_refine.ls_d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' *R* factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine.ls_R_factor_R_work** (alternate). **[refine]**

**_refine.occupancy_max** (*float*)

The maximum value for occupancy found in the coordinate set.

The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.occupancy_min** (*float*)

The minimum value for occupancy found in the coordinate set.

The permitted range is $[0.0, \infty)$. **[refine]**

**_refine.overall_FOM_free_R_set** (*float*)

***_refine.ebi_overall_FOM_free_Rset*** (*ebi_extensions 1.0*)

Average figure of merit of phases of reflections not included in the refinement. This value is derived from the likelihood function

$$\mathrm{FOM} = I_1(X)/I_0(X),$$

where $I_0$, $I_1$ = zero- and first-order modified Bessel functions of the first kind, $X = \sigma_A|E_o||E_c|/\mathrm{SIGMA}$, $E_o, E_c$ = normalized observed and calculated structure factors, $\sigma_A = \langle \cos 2\pi s\delta_x \rangle \sqrt{(\Sigma_P/\Sigma_N)}$ estimated using maximum likelihood, $\Sigma_P = \sum_{\text{atoms in model}} f^2$, $\Sigma_N = \sum_{\text{atoms in crystal}} f^2$, $f$ = form factor of atoms, $\delta_x$ = expected error, $\mathrm{SIGMA} = (\sigma_{\{\mathrm{E;exp}\}})^2 + \varepsilon[1 - (\sigma_A)^2]$, $\sigma_{\{\mathrm{E;exp}\}}$ = uncertainties of normalized observed structure factors and $\varepsilon$ = multiplicity of the diffracting plane.

Reference: Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). *Acta Cryst.* D**53**, 240–255.

**[refine]**

**_refine.overall_FOM_work_R_set** (*float*)

***_refine.ebi_overall_FOM_work_Rset*** (*ebi_extensions 1.0*)

Average figure of merit of phases of reflections included in the refinement. This value is derived from the likelihood function

$$\mathrm{FOM} = I_1(X)/I_0(X),$$

where $I_0$, $I_1$ = zero- and first-order modified Bessel functions of the first kind, $X = \sigma_A|E_o||E_c|/\mathrm{SIGMA}$, $E_o, E_c$ = normalized observed and calculated structure factors, $\sigma_A = \langle \cos 2\pi s\delta_x \rangle \sqrt{(\Sigma_P/\Sigma_N)}$ estimated using maximum likelihood, $\Sigma_P = \sum_{\text{atoms in model}} f^2$, $\Sigma_N = \sum_{\text{atoms in crystal}} f^2$, $f$ = form factor of atoms, $\delta_x$ = expected error, $\mathrm{SIGMA} = (\sigma_{\{\mathrm{E;exp}\}})^2 + \varepsilon[1 - (\sigma_A)^2]$, $\sigma_{\{\mathrm{E;exp}\}}$ = uncertainties of normalized observed structure factors and $\varepsilon$ = multiplicity of the diffracting plane.

Reference: Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). *Acta Cryst.* D**53**, 240–255.

**[refine]**

**_refine.overall_SU_B** (*float*)

***_refine.ebi_Overall_ESU_B*** (*ebi_extensions 1.0*)

The overall standard uncertainty (estimated standard deviation) of the displacement parameters based on a maximum-likelihood residual. The overall standard uncertainty $(\sigma_B)^2$ gives an idea of the uncertainty in the *B* values of averagely defined atoms (atoms with *B* values equal to the average *B* value).

$$(\sigma_B)^2 = \frac{8N_a}{\sum_i [1/\Sigma - (E_o)^2(1-m^2)](\mathrm{SUM\_AS})s^4},$$

where $\mathrm{SUM\_AS} = (\sigma_A)^2/\Sigma^2$, $N_a$ = number of atoms, $\Sigma = (\sigma_{\{E;\mathrm{exp}\}})^2 + \varepsilon[1 - (\sigma_A)^2]$, $E_o$ = normalized structure factors, $\sigma_{\{E;\mathrm{exp}\}}$ = experimental uncertainties of normalized structure factors, $\sigma_A = \langle \cos 2\pi s\delta_x \rangle \sqrt{(\Sigma_P/\Sigma_N)}$ estimated using maximum likelihood, $\Sigma_P = \sum_{\text{atoms in model}} f^2$, $\Sigma_N = \sum_{\text{atoms in crystal}} f^2$, $f$ = form factor of atoms, $\delta_x$ = expected error, $m$ = figure of merit of phases of reflections included in the summation, $s$ = reciprocal-space vector and $\varepsilon$ = multiplicity of the diffracting plane; the summation is over all reflections included in refinement.

References: $\sigma_A$ estimation: Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). *Acta Cryst.* D**53**, 240–255. SU ML estimation: Murshudov, G. N. & Dodson, E. J. (1997). *CCP4 Newsletter on Protein Crystallography*, No. 33, January 1997, pp. 31–39. (http://www.ccp4.ac.uk/newsletters/newsletter33/murshudov.html)

**[refine]**

**_refine.overall_SU_ML** (*float*)

***_refine.ebi_Overall_ESU_ML*** (*ebi_extensions 1.0*)

The overall standard uncertainty (estimated standard deviation) of the positional parameters based on a maximum-likelihood residual. The overall standard uncertainty $(\sigma_X)^2$ gives an idea of the uncertainty in the position of averagely defined atoms (atoms with *B* values equal to the average *B* value).

$$(\sigma_X)^2 = \frac{3N_a}{8\pi^2 \sum_i [1/\Sigma - (E_o)^2(1-m^2)](\mathrm{SUM\_AS})s^2},$$

where $\mathrm{SUM\_AS} = (\sigma_A)^2/\Sigma^2$, $N_a$ = number of atoms, $\Sigma = (\sigma_{\{E;\mathrm{exp}\}})^2 + \varepsilon[1 - (\sigma_A)^2]$, $E_o$ = normalized structure factors, $\sigma_{\{E;\mathrm{exp}\}}$ = experimental uncertainties of normalized structure factors, $\sigma_A = \langle \cos 2\pi s\delta_x \rangle \sqrt{(\Sigma_P/\Sigma_N)}$ estimated using maximum likelihood, $\Sigma_P = \sum_{\text{atoms in model}} f^2$, $\Sigma_N = \sum_{\text{atoms in crystal}} f^2$, $f$ = form factor of atoms, $\delta_x$ = expected error, $m$ = figure of merit of phases of reflections included in the summation, $s$ = reciprocal-space vector and $\varepsilon$ = multiplicity of the diffracting plane; the summation is over all reflections included in refinement.

References: $\sigma_A$ estimation: Murshudov, G. N., Vagin, A. A. & Dodson, E. J. (1997). *Acta Cryst.* D**53**, 240–255. SU ML estimation: Murshudov, G. N. & Dodson, E. J. (1997). *CCP4 Newsletter on Protein Crystallography*, No. 33, January 1997, pp. 31–39. (http://www.ccp4.ac.uk/newsletters/newsletter33/murshudov.html)

**[refine]**

**_refine.overall_SU_R_Cruickshank_DPI** (*float*)
**_refine.ebi_Overall_ESU_R_Cruickshanks_DPI** (*ebi_extensions 1.0*)
The overall standard uncertainty (estimated standard deviation) of the displacement parameters based on the crystallographic *R* value, expressed in a formalism known as the dispersion precision indicator (DPI). The overall standard uncertainty ($\sigma_B$) gives an idea of the uncertainty in the *B* values of averagely defined atoms (atoms with *B* values equal to the average *B* value).

$$(\sigma_B)^2 = 0.65\frac{N_a}{(N_o - N_p)}(R_{\text{value}})^2(D_{\text{min}})^2C^{(-2/3)},$$

where $N_a$ = number of atoms, $N_o$ = number of reflections included in refinement, $N_p$ = number of refined parameters, $R_{\text{value}}$ = conventional crystallographic *R* value, $D_{\text{min}}$ = maximum resolution and *C* = completeness of data.

References: Cruickshank, D. W. J. (1999). *Acta Cryst.* D**55**, 583–601; Murshudov, G. N. & Dodson, E. J. (1997). *CCP4 Newsletter on Protein Crystallography*, No. 33, January 1997, pp. 31–39. (http://www.ccp4.ac.uk/newsletters/newsletter33/murshudov.html)

**[refine]**

**_refine.overall_SU_R_free** (*float*)
**_refine.ebi_Overall_ESU_Rfree** (*ebi_extensions 1.0*)
The overall standard uncertainty (estimated standard deviation) of the displacement parameters based on the free *R* value. The overall standard uncertainty gives an idea of the uncertainty in the *B* values of averagely defined atoms (atoms with *B* values equal to the average *B* value).

$$(\sigma_B)^2 = 0.65\frac{N_a}{N_o}(R_{\text{free}})^2(D_{\text{min}})^2C^{(-2/3)},$$

where $N_a$ = number of atoms, $N_o$ = number of reflections included in the refinement, $R_{\text{free}}$ = conventional free crystallographic *R* value calculated using the reflections not included in the refinement, $D_{\text{min}}$ = maximum resolution and *C* = completeness of data.

References: Cruickshank, D. W. J. (1999). *Acta Cryst.* D**55**, 583–601; Murshudov, G. N. & Dodson, E. J. (1997). *CCP4 Newsletter on Protein Crystallography*, No. 33, January 1997, pp. 31–39. (http://www.ccp4.ac.uk/newsletters/newsletter33/murshudov.html)

**[refine]**

**_refine.solvent_model_details** (*text*)
Special aspects of the solvent model used during refinement.

**[refine]**

**_refine.solvent_model_param_bsol** (*float*)
The value of the $B_{\text{SOL}}$ solvent-model parameter describing the average isotropic displacement parameter of disordered solvent atoms. This is one of the two parameters (the other is **_refine.solvent_model_param_ksol**) in Tronrud's method of modelling the contribution of bulk solvent to the scattering. The standard scale factor is modified according to the expression

$$k_0 \exp(-B_0 s^2)[1 - K_{\text{SOL}} \exp(-B_{\text{SOL}} s^2)],$$

where $k_0$ and $B_0$ are the scale factors for the protein.

Reference: Tronrud, D. E. (1997). *Methods Enzymol.* **277**, 243–268.

**[refine]**

**_refine.solvent_model_param_ksol** (*float*)
The value of the $K_{\text{SOL}}$ solvent-model parameter describing the ratio of the electron density in the bulk solvent to the electron density in the molecular solute. This is one of the two parameters (the other is **_refine.solvent_model_param_bsol**) in Tronrud's method of modelling the contribution of bulk solvent to the scattering. The standard scale factor is modified according to the expression

$$k_0 \exp(-B_0 s^2)[1 - K_{\text{SOL}} \exp(-B_{\text{SOL}} s^2)],$$

where $k_0$ and $B_0$ are the scale factors for the protein.

Reference: Tronrud, D. E. (1997). *Methods Enzymol.* **277**, 243–268.

**[refine]**

## REFINE_ANALYZE

Data items in the REFINE_ANALYZE category record details about the refined structure that are often used to analyze the refinement and assess its quality. A given computer program may or may not produce values corresponding to these data names.

Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_analyze.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_refine_analyze.entry_id
_refine_analyze.Luzzati_coordinate_error_obs
_refine_analyze.Luzzati_d_res_low_obs
       5HVP 0.056  2.51
```

* **_refine_analyze.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**[refine_analyze]**

**_refine_analyze.Luzzati_coordinate_error_free** (*float*)
The estimated coordinate error obtained from the plot of the *R* value *versus* $\sin(\theta)/\lambda$ for the reflections treated as a test set during refinement.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_coordinate_error_obs** (*float*)
The estimated coordinate error obtained from the plot of the *R* value *versus* $\sin(\theta)/\lambda$ for reflections classified as observed.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_d_res_low_free** (*float*)
The value of the low-resolution cutoff used in constructing the Luzzati plot for reflections treated as a test set during refinement.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_d_res_low_obs** (*float*)
The value of the low-resolution cutoff used in constructing the Luzzati plot for reflections classified as observed.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_sigma_a_free** (*float*)
The value of $\sigma_a$ used in constructing the Luzzati plot for the reflections treated as a test set during refinement. Details of the estimation of $\sigma_a$ can be specified in **_refine_analyze.Luzzati_sigma_a_free_details**.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_sigma_a_free_details** (*text*)
Details of the estimation of $\sigma_a$ for the reflections treated as a test set during refinement.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_sigma_a_obs** (*float*)
The value of $\sigma_a$ used in constructing the Luzzati plot for reflections classified as observed. Details of the estimation of $\sigma_a$ can be specified in **_refine_analyze.Luzzati_sigma_a_obs_details**.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.Luzzati_sigma_a_obs_details** (*text*)
Special aspects of the estimation of $\sigma_a$ for the reflections classified as observed.

Reference: Luzzati, V. (1952). *Acta Cryst.* **5**, 802–810.

**[refine_analyze]**

**_refine_analyze.number_disordered_residues** (*float*)
The number of discretely disordered residues in the refined model.

**[refine_analyze]**

**_refine_analyze.occupancy_sum_hydrogen** (*float*)
The sum of the occupancies of the hydrogen atoms in the refined model.

**[refine_analyze]**

**_refine_analyze.occupancy_sum_non_hydrogen** (*float*)
The sum of the occupancies of the non-hydrogen atoms in the refined model.

**[refine_analyze]**

**_refine_analyze.RG_d_res_high** (*float*)
***_refine_analyze.ebi_RG_d_res_high*** (*ebi_extensions 1.0*)
The value of the high-resolution cutoff in ångströms used in the calculation of the Hamilton generalized $R$ factor ($R_G$) stored in **_refine_analyze.RG_work** and **_refine_analyze.RG_free**.

Reference: Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502–510.

The permitted range is $[0.0, \infty)$. **[refine_analyze]**

**_refine_analyze.RG_d_res_low** (*float*)
***_refine_analyze.ebi_RG_d_res_low*** (*ebi_extensions 1.0*)
The value of the low-resolution cutoff in ångströms used in the calculation of the Hamilton generalized R factor ($R_G$) stored in **_refine_analyze.RG_work** and **_refine_analyze.RG_free**.

Reference: Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502–510.

The permitted range is $[0.0, \infty)$. **[refine_analyze]**

**_refine_analyze.RG_free** (*float*)
***_refine_analyze.ebi_RG_free*** (*ebi_extensions 1.0*)
The Hamilton generalized $R$ factor for all reflections that satisfy the resolution limits established by **_refine_analyze.RG_d_res_high** and **_refine_analyze.RG_d_res_low** for the free $R$ set of reflections that were excluded from the refinement.

$$R_G = \sqrt{\frac{\sum_i \sum_j w_{i,j}(|F_{\rm obs}|_i - G|F_{\rm calc}|_i)(|F_{\rm obs}|_j - G|F_{\rm calc}|_j)}{\sum_i \sum_j w_{i,j}|F_{\rm obs}|_i|F_{\rm obs}|_j}},$$

where $|F_{\rm obs}|$ = the observed structure-factor amplitudes, $|F_{\rm calc}|$ = the calculated structure-factor amplitudes, $G$ = the scale factor which puts $|F_{\rm calc}|$ on the same scale as $|F_{\rm obs}|$ and $w_{i,j}$ = the weight for the combination of the reflections $i$ and $j$; $\sum_i$ and $\sum_j$ are taken over the specified reflections.

When the covariance of the amplitudes of reflection $i$ and reflection $j$ is zero (*i.e.* the reflections are independent), $w_{i,i}$ can be redefined as $w_i$ and the nested sums collapsed into one sum:

$$R_G = \sqrt{\frac{\sum_i w_i(|F_{\rm obs}|_i - G|F_{\rm calc}|_i)^2}{\sum_i w_i|F_{\rm obs}|_i^2}}.$$

Reference: Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502–510.

The permitted range is $[0.0, \infty)$. **[refine_analyze]**

**_refine_analyze.RG_free_work_ratio** (*float*)
***_refine_analyze.ebi_RG_work_free_ratio*** (*ebi_extensions 1.0*)
The observed ratio of $R_{G\rm free}$ to $R_{G\rm work}$. The expected $R_G$ ratio is the value that should be achievable at the end of a structure refinement when only random uncorrelated errors exist in the data and the model provided that the observations are properly weighted. When compared with the observed $R_G$ ratio, it may indicate that a structure has not reached convergence or a model has been overrefined with no corresponding improvement in the model.

In an unrestrained refinement, the ratio of $R_{G\rm free}$ to $R_{G\rm work}$ with only random uncorrelated errors at convergence depends only on the number of reflections and the number of parameters according to

$$\sqrt{(f+m)/(f-m)},$$

where $f$ = the number of included structure amplitudes and target distances and $m$ = the number of parameters being refined.

In the restrained case, $R_{G\rm free}$ is calculated from a random selection of residuals including both the structure amplitudes and the restraints. When restraints are included in the refinement, the $R_G$ ratio requires a term for the contribution to the minimized residual at convergence, $D_{\rm restr}$, due to those restraints:

$$D_{\rm restr} = r - \sum[w_i \cdot (a_i)^t \cdot (H)^{-1} a_i],$$

where $r$ is the number of geometrical, displacement-parameter and other restraints, $H$ is the $(m,m)$ normal matrix given by $A^t \cdot W \cdot A$, $W$ is the $(n,n)$ symmetric weight matrix of the included observations, $A$ is the least-squares design matrix of derivatives of order $(n,m)$ and $a_i$ is the $i$th row of $A$. Then the expected $R_G$ ratio becomes

$$\sqrt{[f + (m - r + D_{\rm restr})]/[f - (m - r + D_{\rm restr})]}.$$

There is no data name for the expected value of $R_{G\rm free}/R_{G\rm work}$ yet.

Reference: Tickle, I. J., Laskowski, R. A. & Moss, D. S. (1998). *Acta Cryst.* D**54**, 547–557.

The permitted range is $[0.0, \infty)$. **[refine_analyze]**

**_refine_analyze.RG_work** (*float*)
***_refine_analyze.ebi_RG_work*** (*ebi_extensions 1.0*)
The Hamilton generalized *R* factor for all reflections that satisfy the resolution limits established by **_refine_analyze.RG_d_res_high** and **_refine_analyze.RG_d_res_low** and for those reflections included in the working set when a free *R* set of reflections is omitted from the refinement.

$$R_G = \sqrt{\frac{\sum_i \sum_j w_{i,j}(|F_{\rm obs}|_i - G|F_{\rm calc}|_i)(|F_{\rm obs}|_j - G|F_{\rm calc}|_j)}{\sum_i \sum_j w_{i,j}|F_{\rm obs}|_i|F_{\rm obs}|_j}},$$

where $|F_{\rm obs}|$ = the observed structure-factor amplitudes, $|F_{\rm calc}|$ = the calculated structure-factor amplitudes, $G$ = the scale factor which puts $|F_{\rm calc}|$ on the same scale as $|F_{\rm obs}|$ and $w_{i,j}$ = the weight for the combination of the reflections $i$ and $j$; $\sum_i$ and $\sum_j$ are taken over the specified reflections.

When the covariance of the amplitudes of reflection $i$ and reflection $j$ is zero (*i.e.* the reflections are independent), $w_{i,i}$ can be redefined as $w_i$ and the nested sums collapsed into one sum:

$$R_G = \sqrt{\frac{\sum_i w_i(|F_{\rm obs}|_i - G|F_{\rm calc}|_i)^2}{\sum_i w_i|F_{\rm obs}|_i^2}}.$$

Reference: Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502–510.
The permitted range is $[0.0, \infty)$. **[refine_analyze]**

## REFINE_B_ISO

Data items in the REFINE_B_ISO category record details about the treatment of isotropic *B* factors (displacement parameters) during refinement.
Category group(s): **inclusive_group**, **refine_group**
Category key(s): **_refine_B_iso.class**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_refine_B_iso.class
_refine_B_iso.treatment
 'protein'    isotropic
 'solvent'    isotropic
 'inhibitor'  isotropic
```

***_refine_B_iso.class** (*text*)
A class of atoms treated similarly for isotropic *B*-factor (displacement-parameter) refinement.
Examples: 'all', 'protein', 'solvent', 'sugar-phosphate backbone'.
**[refine_B_iso]**

**_refine_B_iso.details** (*text*)
A description of special aspects of the isotropic *B*-factor (displacement-parameter) refinement for the class of atoms described in **_refine_B_iso.class**.
Example:
```
; The temperature factors of atoms in the side chain of Arg 92
were held fixed due to unstable behavior in refinement.
;
```
**[refine_B_iso]**

**_refine_B_iso.treatment** (*ucode*)
The treatment of isotropic *B*-factor (displacement-parameter) refinement for a class of atoms defined in **_refine_B_iso.class**.
The data value must be one of the following:
fixed
isotropic
anisotropic
**[refine_B_iso]**

**_refine_B_iso.value** (*float*)
The value of the isotropic *B* factor (displacement parameter) assigned to a class of atoms defined in **_refine_B_iso.class**. Meaningful only for atoms with fixed isotropic *B* factors.
**[refine_B_iso]**

## REFINE_FUNCT_MINIMIZED

Data items in the REFINE_FUNCT_MINIMIZED category record details about the individual terms of the function minimized during refinement.
Category group(s): **inclusive_group**, **refine_group**
Category key(s): **_refine_funct_minimized.type**

*Example 1 – based on RESTRAIN refinement for the CCP4 test data set toxd.*

```
loop_
_refine_funct_minimized.type
_refine_funct_minimized.number_terms
_refine_funct_minimized.residual
'sum(W*Delta(Amplitude)^2'                3009      1621.3
'sum(W*Delta(Plane+Rigid)^2'                85       56.68
'sum(W*Delta(Distance)^2'                 1219      163.59
'sum(W*Delta(U-tempfactors)^2'            1192      69.338
```

**_refine_funct_minimized.number_terms** (*int*)
***_ebi_refine_funct_minimized.NumTerms*** (*ebi_extensions 1.0*)
The number of observations in this term. For example, if the term is a residual of the X-ray intensities, this item would contain the number of reflections used in the refinement.
The permitted range is $[0, \infty)$. **[refine_funct_minimized]**

**_refine_funct_minimized.residual** (*float*)
***_ebi_refine_funct_minimized.Residual*** (*ebi_extensions 1.0*)
The residual for this term of the function that was minimized during the refinement.
The permitted range is $[0.0, \infty)$. **[refine_funct_minimized]**

***_refine_funct_minimized.type** (*line*)
***_ebi_refine_funct_minimized.type*** (*ebi_extensions 1.0*)
The type of the function being minimized.
**[refine_funct_minimized]**

**_refine_funct_minimized.weight** (*float*)
***_ebi_refine_funct_minimized.weight*** (*ebi_extensions 1.0*)
The weight applied to this term of the function that was minimized during the refinement.
**[refine_funct_minimized]**

## REFINE_HIST

Data items in the REFINE_HIST category record details about the steps during the refinement of the structure. These data items are not meant to be as thorough a description of the refinement as is provided for the final model in other categories; rather, these data items provide a mechanism for sketching out the progress of the refinement, supported by a small set of representative statistics.
Category group(s): **inclusive_group**, **refine_group**
Category key(s): **_refine_hist.cycle_id**

*Example 1 – based on laboratory records for the collagen-like peptide [(POG)$_4$ EKG (POG)$_5$]$_3$.*

```
_refine_hist.cycle_id                C134
_refine_hist.d_res_high              1.85
_refine_hist.d_res_low               20.0
_refine_hist.number_atoms_solvent     217
_refine_hist.number_atoms_total       808
_refine_hist.number_reflns_all       6174
_refine_hist.number_reflns_obs       4886
_refine_hist.number_reflns_R_free     476
_refine_hist.number_reflns_R_work    4410
_refine_hist.R_factor_all            .265
_refine_hist.R_factor_obs            .195
_refine_hist.R_factor_R_free         .274
_refine_hist.R_factor_R_work         .160
_refine_hist.details
; Add majority of solvent molecules. B factors refined by
  group. Continued to remove misplaced water molecules.
;
```

* **_refine_hist.cycle_id** (*code*)
The value of **_refine_hist.cycle_id** must uniquely identify a record in the REFINE_HIST list. Note that this item need not be a number; it can be any unique identifier.

**[refine_hist]**

* **_refine_hist.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data for this cycle of refinement. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[refine_hist]**

* **_refine_hist.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data for this cycle of refinement. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[refine_hist]**

**_refine_hist.details** (*text*)
A description of special aspects of this cycle of the refinement process.
Example:
```
; Residues 13-17 fit and added to model; substantial
rebuilding of loop containing residues 43-48; addition of
first atoms to solvent model; ten cycles of Prolsq refinement.
;
```
**[refine_hist]**

**_refine_hist.number_atoms_solvent** (*int*)
The number of solvent atoms that were included in the model at this cycle of the refinement.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.number_atoms_total** (*int*)
The total number of atoms that were included in the model at this cycle of the refinement.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.number_reflns_all** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low**.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.number_reflns_obs** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.number_reflns_R_free** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.number_reflns_R_work** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine_hist]**

**_refine_hist.R_factor_all** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes and $F_{\rm calc}$ = the calculated structure-factor amplitudes; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine_hist]**

**_refine_hist.R_factor_obs** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes and $F_{\rm calc}$ = the calculated structure-factor amplitudes; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine_hist]**

**_refine_hist.R_factor_R_free** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes and $F_{\rm calc}$ = the calculated structure-factor amplitudes; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$. **[refine_hist]**

**_refine_hist.R_factor_R_work** (*float*)

Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_hist.d_res_high** and **_refine_hist.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes and $F_{\rm calc}$ = the calculated structure-factor amplitudes; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$. **[refine_hist]**

## REFINE_LS_CLASS

Data items in the REFINE_LS_CLASS category record details about the reflections used for the structure refinement for each reflection class separately.

Category key(s): **_refine_ls_class.code**

*Example 1 – data for a modulated structure from van Smaalen [J. Phys. Condens. Matter (1991), **3**, 1247–1263].*

```
loop_
  _refine_ls_class.R_factor_gt
  _refine_ls_class.code
      0.057    'Main'
      0.074    'Com'
      0.064    'NbRefls'
      0.046    'LaRefls'
      0.112    'Sat1'
      0.177    'Sat2'
```

* **_refine_ls_class.code** (*code*)

***_refine_ls_class_code*** (*cif_core.dic 2.3*)

The code identifying a certain reflection class. This code must match a **_reflns_class.code**.

Examples: '1', 'm1', 's2'. **[refine_ls_class]**

**_refine_ls_class.d_res_high** (*float*)

***_refine_ls_class_d_res_high*** (*cif_core.dic 2.3*)

For each reflection class, the lowest value in ångströms for the interplanar spacings for the reflections used in the refinement. This is called the highest resolution.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.d_res_low** (*float*)

***_refine_ls_class_d_res_low*** (*cif_core.dic 2.3*)

For each reflection class, the highest value in ångströms for the interplanar spacings for the reflections used in the refinement. This is called the lowest resolution.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.R_factor_all** (*float*)

***_refine_ls_class_R_factor_all*** (*cif_core.dic 2.3*)

For each reflection class, the residual factor for all reflections satisfying the resolution limits established by **_refine_ls_class.d_res_high** and **_refine_ls_class.d_res_low**. This is the conventional $R$ factor. See also the definition of **_refine_ls_class.wR_factor_all**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.R_factor_gt** (*float*)

***_refine_ls_class_R_factor_gt*** (*cif_core.dic 2.3*)

For each reflection class, the residual factor for significantly intense reflections (see **_reflns.threshold_expression**) included in the refinement. The reflections also satisfy the resolution limits established by **_refine_ls_class.d_res_high** and **_refine_ls_class.d_res_low**. This is the conventional $R$ factor. See also the definition of **_refine_ls_class.wR_factor_all**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.R_Fsqd_factor** (*float*)

***_refine_ls_class_R_Fsqd_factor*** (*cif_core.dic 2.3*)

For each reflection class, the residual factor $R(F^2)$ calculated on the squared amplitudes of the observed and calculated structure factors for the reflections judged significantly intense (*i.e.* satisfying the threshold specified by **_reflns.threshold_expression**) and included in the refinement. The reflections also satisfy the resolution limits established by **_refine_ls_class.d_res_high** and **_refine_ls_class.d_res_low**.

$$R(F^2) = \frac{\sum |F^2_{\rm obs} - F^2_{\rm calc}|}{\sum |F^2_{\rm obs}|},$$

where $F^2_{\rm obs}$ = squares of the observed structure-factor amplitudes, $F^2_{\rm calc}$ = squares of the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.R_I_factor** (*float*)

***_refine_ls_class_R_I_factor*** (*cif_core.dic 2.3*)

For each reflection class, the residual factor $R(I)$ for the reflections judged significantly intense (*i.e.* satisfying the threshold specified by **_reflns.threshold_expression**) and included in the refinement. This is most often calculated in Rietveld refinements against powder data, where it is referred to as $R_B$ or $R_{\rm Bragg}$.

$$R(I) = \frac{\sum |I_{\rm obs} - I_{\rm calc}|}{\sum |I_{\rm obs}|},$$

where $I_{\rm obs}$ = the net observed intensities, $I_{\rm calc}$ = the net calculated intensities and the sum is taken over the reflections of this class.

The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

**_refine_ls_class.wR_factor_all** (*float*)
***_refine_ls_class_wR_factor_all*** (*cif_core.dic 2.3*)
For each reflection class, the weighted residual factor for all reflections included in the refinement. The reflections also satisfy the resolution limits established by **_refine_ls_class.d_res_high** and **_refine_ls_class.d_res_low**. See also the **_refine_ls_class.R_factor_** definitions.

$$wR = \left( \frac{\sum |w|Y_{\rm obs} - Y_{\rm calc}|^2|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitudes specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitudes specified by **_refine.ls_structure_factor_coef**, $w$ = the least-squares weight and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[refine_ls_class]**

## REFINE_LS_RESTR

Data items in the REFINE_LS_RESTR category record details about the restraints applied to various classes of parameters during the least-squares refinement.
Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_ls_restr.type**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_refine_ls_restr.type
_refine_ls_restr.dev_ideal_target
_refine_ls_restr.dev_ideal
_refine_ls_restr.number
_refine_ls_restr.criterion
_refine_ls_restr.rejects
 'p_bond_d'           0.020  0.018  1654  '> 2\s'  22
 'p_angle_d'          0.030  0.038  2246  '> 2\s'  139
 'p_planar_d'         0.040  0.043  498   '> 2\s'  21
 'p_planar'           0.020  0.015  270   '> 2\s'  1
 'p_chiral'           0.150  0.177  278   '> 2\s'  2
 'p_singtor_nbd'      0.500  0.216  582   '> 2\s'  0
 'p_multtor_nbd'      0.500  0.207  419   '> 2\s'  0
 'p_xyhbond_nbd'      0.500  0.245  149   '> 2\s'  0
 'p_planar_tor'       3.0    2.6    203   '> 2\s'  9
 'p_staggered_tor'    15.0   17.4   298   '> 2\s'  31
 'p_orthonormal_tor'  20.0   18.1   12    '> 2\s'  1
```

**_refine_ls_restr.criterion** (*text*)
A criterion used to define a parameter value that deviates significantly from its ideal value in the model obtained by restrained least-squares refinement.
Example: '> 3\s'. **[refine_ls_restr]**

**_refine_ls_restr.dev_ideal** (*float*)
For the given parameter type, the root-mean-square deviation between the ideal values used as restraints in the least-squares refinement and the values obtained by refinement. For instance, bond distances may deviate by 0.018 Å (r.m.s.) from ideal values in the current model.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr]**

**_refine_ls_restr.dev_ideal_target** (*float*)
For the given parameter type, the target root-mean-square deviation between the ideal values used as restraints in the least-squares refinement and the values obtained by refinement.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr]**

**_refine_ls_restr.number** (*int*)
The number of parameters of this type subjected to restraint in least-squares refinement.
The permitted range is $[0, \infty)$. **[refine_ls_restr]**

**_refine_ls_restr.rejects** (*int*)
The number of parameters of this type that deviate from ideal values by more than the amount defined in **_refine_ls_restr.criterion** in the model obtained by restrained least-squares refinement.
The permitted range is $[0, \infty)$. **[refine_ls_restr]**

***_refine_ls_restr.type** (*line*)
The type of the parameter being restrained. Explicit sets of data values are provided for the programs *PROTIN/PROLSQ* (beginning with *p_*) and *RESTRAIN* (beginning with *RESTRAIN_*). As computer programs change, these data values are given as examples, not as an enumeration list. Computer programs that convert a data block to a refinement table will expect the exact form of the data values given here to be used.
*The following item(s) have an equivalent role in their respective categories:*
***_refine_ls_restr_type.type***.
Examples: 'p_bond_d' (bond distance), 'p_angle_d' (bond angle expressed as a distance), 'p_planar_d' (planar 1,4 distance), 'p_xhbond_d' (*X*—H bond distance), 'p_xhangle_d' (*X*—H bond angle expressed as a distance), 'p_hydrog_d' (hydrogen distance), 'p_special_d' (special distance), 'p_planar' (planes), 'p_chiral' (chiral centres), 'p_singtor_nbd' (single-torsion non-bonded contact), 'p_multtor_nbd' (multiple-torsion non-bonded contact), 'p_xyhbond_nbd' (possible $X\cdots Y$ hydrogen bond), 'p_xhyhbond_nbd' (possible *X*—H$\cdots Y$ hydrogen bond), 'p_special_tor' (special torsion angle), 'p_planar_tor' (planar torsion angle), 'p_staggered_tor' (staggered torsion angle), 'p_orthonormal_tor' (orthonormal torsion angle), 'p_mcbond_it' (main-chain bond isotropic displacement parameter), 'p_mcangle_it' (main-chain angle isotropic displacement parameter), 'p_scbond_it' (side-chain bond isotropic displacement parameter), 'p_scangle_it' (side-chain angle isotropic displacement parameter), 'p_xhbond_it' (*X*—H bond isotropic displacement parameter), 'p_xhangle_it' (*X*—H angle isotropic displacement parameter), 'p_special_it' (special isotropic displacement parameter), 'RESTRAIN_Distances < 2.12' (the root-mean-square deviation of the difference between the values calculated from the structures used to compile the restraints dictionary parameters and the dictionary values themselves in the distance range less than 2.12 Å), 'RESTRAIN_Distances 2.12 < D < 2.625' (the root-mean-square deviation of the difference between the values calculated from the structures used to compile the restraints dictionary parameters and the dictionary values themselves in the distance range 2.12–2.625 Å), 'RESTRAIN_Distances > 2.625' (the root-mean-square deviation of the difference between the values calculated from the structures used to compile the restraints dictionary parameters and the dictionary values themselves in the distance range greater than 2.625 Å), 'RESTRAIN_Peptide Planes' (the root-mean-square deviation of the difference between the values calculated from the structures used to compile the restraints dictionary parameters and the dictionary values themselves for peptide planes), 'RESTRAIN_Ring and other planes' (the root-mean-square deviation of the difference between the values calculated from the structures used to compile the restraints dictionary parameters and the dictionary values themselves for rings and planes other than peptide planes), 'RESTRAIN_rms diffs for Uiso atoms at dist 1.2-1.4', 'RESTRAIN_rms diffs for Uiso atoms at dist 1.4-1.6', 'RESTRAIN_rms diffs for Uiso atoms at dist 1.8-2.0', 'RESTRAIN_rms diffs for Uiso atoms at dist 2.0-2.2', 'RESTRAIN_rms diffs for Uiso atoms at dist 2.2-2.4', 'RESTRAIN_rms diffs for Uiso atoms at dist >2.4'.
**[refine_ls_restr]**

**_refine_ls_restr.weight** (*float*)
The weighting value applied to this type of restraint in the least-squares refinement.
**[refine_ls_restr]**

## REFINE_LS_RESTR_NCS

Data items in the REFINE_LS_RESTR_NCS category record details about the restraints applied to atom positions in domains related by noncrystallographic symmetry during least-squares refinement, and also about the deviation of the restrained atomic parameters at the end of the refinement. It is expected that these values will only be reported once for each set of restrained domains.

Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_ls_restr_ncs.dom_id**

*Example 1 – based on laboratory records for the collagen-like peptide, HYP-.*

```
_refine_ls_restr_ncs.dom_id             d2
_refine_ls_restr_ncs.weight_position    300.0
_refine_ls_restr_ncs.weight_B_iso       2.0
_refine_ls_restr_ncs.rms_dev_position   0.09
_refine_ls_restr_ncs.rms_dev_B_iso      0.16
_refine_ls_restr_ncs.ncs_model_details
;
 NCS restraint for pseudo-twofold symmetry between domains
 d1 and d2.  Position weight coefficient given in
 Kcal/(mol \%A^2^) and isotropic B weight coefficient given
 in \%A^2^.
;
```

* **_refine_ls_restr_ncs.dom_id** (*code*)
This data item is a pointer to **_struct_ncs_dom.id** in the STRUCT_NCS_DOM category.

**[refine_ls_restr_ncs]**

**_refine_ls_restr_ncs.ncs_model_details** (*text*)
Special aspects of the manner in which noncrystallographic restraints were applied to atomic parameters in the domain specified by **_refine_ls_restr_ncs.dom_id** and equivalent atomic parameters in the domains against which it was restrained.

**[refine_ls_restr_ncs]**

**_refine_ls_restr_ncs.rms_dev_B_iso** (*float*)
The root-mean-square deviation in equivalent isotropic displacement parameters in the domain specified by **_refine_ls_restr_ncs.dom_id** and in the domains against which it was restrained.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr_ncs]**

**_refine_ls_restr_ncs.rms_dev_position** (*float*)
The root-mean-square deviation in equivalent atom positions in the domain specified by **_refine_ls_restr_ncs.dom_id** and in the domains against which it was restrained.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr_ncs]**

**_refine_ls_restr_ncs.weight_B_iso** (*float*)
The value of the weighting coefficient used in noncrystallographic symmetry restraint of isotropic displacement parameters in the domain specified by **_refine_ls_restr_ncs.dom_id** to equivalent isotropic displacement parameters in the domains against which it was restrained.

**[refine_ls_restr_ncs]**

**_refine_ls_restr_ncs.weight_position** (*float*)
The value of the weighting coefficient used in noncrystallographic symmetry restraint of atom positions in the domain specified by **_refine_ls_restr_ncs.dom_id** to equivalent atom positions in the domains against which it was restrained.

**[refine_ls_restr_ncs]**

## REFINE_LS_RESTR_TYPE

Data items in the REFINE_LS_RESTR_TYPE category record details about the restraint types used in the least-squares refinement.

Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_ls_restr_type.type**

*Example 1 – based on RESTRAIN refinement for the CCP4 test data set toxd.*

```
loop_
_refine_ls_restr.type
_refine_ls_restr.number
_refine_ls_restr.dev_ideal
_refine_ls_restr.dev_ideal_target
 'RESTRAIN Distances < 2.12'              509     0.005 0.022
 'RESTRAIN Distances 2.12 < D < 2.625'    671     0.016 0.037
 'RESTRAIN Distances > 2.625'              39     0.034 0.043
 'RESTRAIN Peptide Planes'                 59     0.002 0.010
 'RESTRAIN Ring and other planes'          26     0.014 0.010
 'RESTRAIN rms diffs for Uiso atoms at dist 1.2-1.4'
     212     0.106   .
 'RESTRAIN rms diffs for Uiso atoms at dist 1.4-1.6'
     288     0.101   .
 'RESTRAIN rms diffs for Uiso atoms at dist 1.8-2.0'
       6     0.077   .
 'RESTRAIN rms diffs for Uiso atoms at dist 2.0-2.2'
      10     0.114   .
 'RESTRAIN rms diffs for Uiso atoms at dist 2.2-2.4'
     215     0.119   .
 'RESTRAIN rms diffs for Uiso atoms at dist >2.4'
     461     0.106   .

loop_
_refine_ls_restr_type.type
_refine_ls_restr_type.distance_cutoff_low
_refine_ls_restr_type.distance_cutoff_high
 'RESTRAIN Distances < 2.12'                    .     2.12
 'RESTRAIN Distances 2.12 < D < 2.625'       2.12  2.625
 'RESTRAIN Distances > 2.625'                2.625 .
 'RESTRAIN Peptide Planes'                   .     .
 'RESTRAIN Ring and other planes'            .     .
 'RESTRAIN rms diffs for Uiso atoms at dist 1.2-1.4'
     1.2   1.4
 'RESTRAIN rms diffs for Uiso atoms at dist 1.4-1.6'
     1.4   1.6
 'RESTRAIN rms diffs for Uiso atoms at dist 1.8-2.0'
     1.8   2.0
 'RESTRAIN rms diffs for Uiso atoms at dist 2.0-2.2'
     2.0   2.2
 'RESTRAIN rms diffs for Uiso atoms at dist 2.2-2.4'
     2.2   2.4
 'RESTRAIN rms diffs for Uiso atoms at dist >2.4'
     2.4   .
```

**_refine_ls_restr_type.distance_cutoff_high** (*float*)
The upper limit in ångströms of the distance range applied to the current restraint type.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr_type]**

**_refine_ls_restr_type.distance_cutoff_low** (*float*)
The lower limit in ångströms of the distance range applied to the current restraint type.
The permitted range is $[0.0, \infty)$. **[refine_ls_restr_type]**

* **_refine_ls_restr_type.type** (*line*)
This data item is a pointer to **_refine_ls_restr.type** in the REFINE_LS_RESTR category.

**[refine_ls_restr_type]**

## REFINE_LS_SHELL

Data items in the REFINE_LS_SHELL category record details about the results of the least-squares refinement broken down into shells of resolution.

Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_ls_shell.d_res_low**
**_refine_ls_shell.d_res_high**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_refine_ls_shell.d_res_low
_refine_ls_shell.d_res_high
_refine_ls_shell.number_reflns_obs
_refine_ls_shell.R_factor_obs
  8.00   4.51   1226   0.196
  4.51   3.48   1679   0.146
  3.48   2.94   2014   0.160
  2.94   2.59   2147   0.182
  2.59   2.34   2127   0.193
  2.34   2.15   2061   0.203
  2.15   2.00   1647   0.188
```

* **_refine_ls_shell.d_res_high** (*float*)
The lowest value for the interplanar spacings for the reflection data in this shell. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[refine_ls_shell]**

* **_refine_ls_shell.d_res_low** (*float*)
The highest value for the interplanar spacings for the reflection data in this shell. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[refine_ls_shell]**

**_refine_ls_shell.number_reflns_all** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low**.
The permitted range is $[0, \infty)$. **[refine_ls_shell]**

**_refine_ls_shell.number_reflns_obs** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.
The permitted range is $[0, \infty)$. **[refine_ls_shell]**

**_refine_ls_shell.number_reflns_R_free** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' *R* factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine_ls_shell]**

**_refine_ls_shell.number_reflns_R_work** (*int*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' *R* factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.
The permitted range is $[0, \infty)$. **[refine_ls_shell]**

**_refine_ls_shell.percent_reflns_obs** (*float*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion**, expressed as a percentage of the number of geometrically observable reflections that satisfy the resolution limits.
**[refine_ls_shell]**

**_refine_ls_shell.percent_reflns_R_free** (*float*)
The number of reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' *R* factor, expressed as a percentage of the number of geometrically observable reflections that satisfy the reflection limits.
**[refine_ls_shell]**

**_refine_ls_shell.R_factor_all** (*float*)
Residual factor *R* for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low**.

$$R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|},$$

where $F_{\text{obs}}$ = the observed structure-factor amplitudes, $F_{\text{calc}}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine_ls_shell.wR_factor_all** (alternate).
**[refine_ls_shell]**

**_refine_ls_shell.R_factor_obs** (*float*)
Residual factor *R* for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.

$$R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum |F_{\text{obs}}|},$$

where $F_{\text{obs}}$ = the observed structure-factor amplitudes, $F_{\text{calc}}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine_ls_shell.wR_factor_obs** (alternate).
**[refine_ls_shell]**

**_refine_ls_shell.R_factor_R_free** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related items: **_refine_ls_shell.wR_factor_R_free** (alternate), **_refine_ls_shell.R_factor_R_free_error** (associated error).

**[refine_ls_shell]**

**_refine_ls_shell.R_factor_R_free_error** (*float*)
The estimated error in **_refine_ls_shell.R_factor_R_free**. The method used to estimate the error is described in the item **_refine.ls_R_factor_R_free_error_details**.

Related item: **_refine_ls_shell.R_factor_R_free** (associated value).

**[refine_ls_shell]**

**_refine_ls_shell.R_factor_R_work** (*float*)
Residual factor $R$ for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine_ls_shell.wR_factor_R_work** (alternate).

**[refine_ls_shell]**

**_refine_ls_shell.redundancy_reflns_all** (*float*)
The ratio of the total number of observations of the reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** to the number of crystallographically unique reflections that satisfy the same limits.

**[refine_ls_shell]**

**_refine_ls_shell.redundancy_reflns_obs** (*float*)
The ratio of the total number of observations of the reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion** to the number of crystallographically unique reflections that satisfy the same limits.

**[refine_ls_shell]**

**_refine_ls_shell.wR_factor_all** (*float*)
Weighted residual factor $wR$ for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine_ls_shell.R_factor_all** (alternate).

**[refine_ls_shell]**

**_refine_ls_shell.wR_factor_obs** (*float*)
Weighted residual factor $wR$ for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine_ls_shell.R_factor_obs** (alternate).

**[refine_ls_shell]**

**_refine_ls_shell.wR_factor_R_free** (*float*)
Weighted residual factor $wR$ for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the test reflections (*i.e.* were excluded from the refinement) when the refinement included the calculation of a 'free' $R$ factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.

The permitted range is $[0.0, \infty)$.

Related item: **_refine_ls_shell.R_factor_R_free** (alternate).

**[refine_ls_shell]**

**_refine_ls_shell.wR_factor_R_work** (*float*)
Weighted residual factor *wR* for reflections that satisfy the resolution limits established by **_refine_ls_shell.d_res_high** and **_refine_ls_shell.d_res_low** and the observation limit established by **_reflns.observed_criterion**, and that were used as the working reflections (*i.e.* were included in the refinement) when the refinement included the calculation of a 'free' *R* factor. Details of how reflections were assigned to the working and test sets are given in **_reflns.R_free_details**.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY_{\rm obs}^2|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef** and $w$ = the least-squares weight; the sum is taken over the specified reflections.
The permitted range is $[0.0, \infty)$.
Related item: **_refine_ls_shell.R_factor_R_work** (alternate).
**[refine_ls_shell]**

**REFINE_OCCUPANCY**

Data items in the REFINE_OCCUPANCY category record details about the treatment of atom occupancies during refinement.
Category group(s): **inclusive_group**
**refine_group**
Category key(s): **_refine_occupancy.class**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_refine_occupancy.class
_refine_occupancy.treatment
_refine_occupancy.value
_refine_occupancy.details
 'protein'                  fix  1.00  .
 'solvent'                  fix  1.00  .
 'inhibitor orientation 1'  fix  0.65  .
 'inhibitor orientation 2'  fix  0.35
; The inhibitor binds to the enzyme in two alternative
  conformations. The occupancy of each conformation was
  adjusted so as to result in approximately equal mean
  thermal factors for the atoms in each conformation.
;
```

***_refine_occupancy.class** (*text*)
The class of atoms treated similarly for occupancy refinement.
Examples: 'all', 'protein', 'solvent', 'sugar-phosphate backbone'.
**[refine_occupancy]**

**_refine_occupancy.details** (*text*)
A description of special aspects of the occupancy refinement for a class of atoms described in **_refine_occupancy.class**.
Example:

```
; The inhibitor binds to the enzyme in two alternative
conformations. The occupancy of each conformation was
adjusted so as to result in approximately equal mean thermal
factors for the atoms in each conformation.
;
```

**[refine_occupancy]**

**_refine_occupancy.treatment** (*ucode*)
The treatment of occupancies for a class of atoms described in **_refine_occupancy.class**.
The data value must be one of the following:
fix fixed
ref refined
**[refine_occupancy]**

**_refine_occupancy.value** (*float*)
The value of occupancy assigned to a class of atoms defined in **_refine_occupancy.class**. Meaningful only for atoms with fixed occupancy.
The permitted range is [0.0, 1.0].
Examples: '1.0', '0.41'.
**[refine_occupancy]**

**REFLN**

Data items in the REFLN category record details about the reflection data used to determine the ATOM_SITE data items. The REFLN data items refer to individual reflections and must be included in looped lists. The REFLNS data items specify the parameters that apply to all reflections. The REFLNS data items are not looped.
Category group(s): **inclusive_group**
**refln_group**
Category key(s): **_refln.index_h**
**_refln.index_k**
**_refln.index_l**

*Example 1 – based on data set fetod of Todres, Yanovsky, Ermekov & Struchkov [Acta Cryst. (1993), C**49**, 1352–1354].*

```
loop_
_refln.index_h
_refln.index_k
_refln.index_l
_refln.F_squared_calc
_refln.F_squared_meas
_refln.F_squared_sigma
_refln.status
   2   0   0       85.57       58.90      1.45 o
   3   0   0    15718.18    15631.06     30.40 o
   4   0   0    55613.11    49840.09     61.86 o
   5   0   0      246.85      241.86     10.02 o
   6   0   0       82.16       69.97      1.93 o
   7   0   0     1133.62      947.79     11.78 o
   8   0   0     2558.04     2453.33     20.44 o
   9   0   0      283.88      393.66      7.79 o
  10   0   0      283.70      171.98      4.26 o
```

**_refln.A_calc** (*float*)
***_refln_A_calc*** (*cif_core.dic 2.0.1*)
The calculated value of structure-factor component *A* in electrons.

$$A = |F| \cos(\text{phase}).$$

Related item: **_refln.A_calc_au** (conversion arbitrary). **[refln]**

**_refln.A_calc_au** (*float*)
The calculated value of structure-factor component *A* in arbitrary units.

$$A = |F| \cos(\text{phase}).$$

Related item: **_refln.A_calc** (conversion arbitrary). **[refln]**

**_refln.A_meas** (*float*)
***_refln_A_meas*** (*cif_core.dic 2.0.1*)
The measured value of structure-factor component *A* in electrons.

$$A = |F| \cos(\text{phase}).$$

Related item: **_refln.A_meas_au** (conversion arbitrary). **[refln]**

**_refln.A_meas_au** (*float*)
The measured value of structure-factor component *A* in arbitrary units.

$$A = |F| \cos(\text{phase}).$$

Related item: **_refln.A_meas** (conversion arbitrary). **[refln]**

**_refln.B_calc** (*float*)
_refln_B_calc (*cif_core.dic 2.0.1*)
The calculated value of structure-factor component $B$ in electrons.

$$B = |F| \sin(\text{phase}).$$

Related item: **_refln.B_calc_au** (conversion arbitrary). **[refln]**

**_refln.B_calc_au** (*float*)
The calculated value of structure-factor component $B$ in arbitrary units.

$$B = |F| \sin(\text{phase}).$$

Related item: **_refln.B_calc** (conversion arbitrary). **[refln]**

**_refln.B_meas** (*float*)
_refln_B_meas (*cif_core.dic 2.0.1*)
The measured value of structure-factor component $B$ in electrons.

$$B = |F| \sin(\text{phase}).$$

Related item: **_refln.B_meas_au** (conversion arbitrary). **[refln]**

**_refln.B_meas_au** (*float*)
The measured value of structure-factor component $B$ in arbitrary units.

$$B = |F| \sin(\text{phase}).$$

Related item: **_refln.B_meas** (conversion arbitrary). **[refln]**

**_refln.class_code** (*code*)
_refln_class_code (*cif_core.dic 2.3*)
The code identifying the class to which this reflection has been assigned. This code must match a value of **_reflns_class.code**. Reflections may be grouped into classes for a variety of purposes. For example, for modulated structures each reflection class may be defined by the number $m = \sum |m_i|$, where the $m_i$ are the integer coefficients that, in addition to $h, k, l$, index the corresponding diffraction vector in the basis defined for the reciprocal lattice.
**[refln]**

*_refln.crystal_id
_refln_crystal_id (*cif_core.dic 2.0.1*)
This data item is a pointer to **_exptl_crystal.id** in the EXPTL_CRYSTAL category.

**_refln.d_spacing** (*float*)
_refln_d_spacing (*cif_core.dic 2.3*)
The $d$ spacing in ångströms for this reflection. This is related to the $(\sin\theta)/\lambda$ value by the expression **_refln.d_spacing** = 2/(**_refln.sint/lambda**).
The permitted range is $[0.0, \infty)$. **[refln]**

**_refln.F_calc** (*float*)
_refln_F_calc (*cif_core.dic 2.0.1*)
The calculated value of the structure factor in electrons.
Related item: **_refln.F_calc_au** (conversion arbitrary). **[refln]**

**_refln.F_calc_au** (*float*)
The calculated value of the structure factor in arbitrary units.
Related item: **_refln.F_calc** (conversion arbitrary). **[refln]**

**_refln.F_meas** (*float, su*)
_refln_F_meas (*cif_core.dic 2.0.1*)
The measured value of the structure factor in electrons.
Related items: **_refln.F_meas_sigma** (associated esd),
**_refln.F_meas_au** (conversion arbitrary). **[refln]**

**_refln.F_meas_au** (*float, su*)
The measured value of the structure factor in arbitrary units.
Related items: **_refln.F_meas_sigma_au** (associated esd),
**_refln.F_meas** (conversion arbitrary). **[refln]**

**_refln.F_meas_sigma** (*float*)
_refln_F_sigma (*cif_core.dic 2.0.1*)
The standard uncertainty (estimated standard deviation) of **_refln.F_meas** in electrons.
Related items: **_refln.F_meas** (associated value),
**_refln.F_meas_sigma_au** (conversion arbitrary). **[refln]**

**_refln.F_meas_sigma_au** (*float*)
The standard uncertainty (estimated standard deviation) of **_refln.F_meas_au** in arbitrary units.
Related items: **_refln.F_meas_au** (associated value),
**_refln.F_meas_sigma** (conversion arbitrary). **[refln]**

**_refln.F_squared_calc** (*float*)
_refln_F_squared_calc (*cif_core.dic 2.0.1*)
The calculated value of the squared structure factor in electrons squared.
**[refln]**

**_refln.F_squared_meas** (*float*)
_refln_F_squared_meas (*cif_core.dic 2.0.1*)
The measured value of the squared structure factor in electrons squared.
**[refln]**

**_refln.F_squared_sigma** (*float*)
_refln_F_squared_sigma (*cif_core.dic 2.0.1*)
The standard uncertainty (derived from measurement) of the squared structure factor in electrons squared.
**[refln]**

**_refln.fom** (*float*)
The figure of merit $m$ for this reflection.

$$m = \frac{\int P_\alpha \exp(i\alpha)\, \mathrm{d}\alpha}{\int P_\alpha\, \mathrm{d}\alpha},$$

where $P_\alpha$ = the probability that the phase angle $\alpha$ is correct; the integral is taken over the range $\alpha = 0$ to $2\pi$.
The permitted range is $[0.0, \infty)$. **[refln]**

**_refln.include_status** (*code*)
_refln_include_status (*cif_core.dic 2.3*)
Classification of a reflection so as to indicate its status with respect to inclusion in the refinement and the calculation of $R$ factors.
Related item: **_refln.status** (alternate).
The data value must be one of the following:

| | |
|---|---|
| o | (lower-case letter o for 'observed') satisfies **_refine.ls_d_res_high**, satisfies **_refine.ls_d_res_low** and exceeds **_reflns.threshold_expression** |
| < | satisfies **_refine.ls_d_res_high**, satisfies **_refine.ls_d_res_low** and does not exceed **_reflns.threshold_expression** |
| - | systematically absent reflection |
| x | unreliable measurement – not used |
| h | does not satisfy **_refine.ls_d_res_high** |
| l | does not satisfy **_refine.ls_d_res_low** |

**[refln]**

*`_refln.index_h` (*int*)
`_refln_index_h` (*cif_core.dic 2.0.1*)
Miller index $h$ of the reflection. The values of the Miller indices in the REFLN category must correspond to the cell defined by cell lengths and cell angles in the CELL category.
**[refln]**

*`_refln.index_k` (*int*)
`_refln_index_k` (*cif_core.dic 2.0.1*)
Miller index $k$ of the reflection. The values of the Miller indices in the REFLN category must correspond to the cell defined by cell lengths and cell angles in the CELL category.
**[refln]**

*`_refln.index_l` (*int*)
`_refln_index_l` (*cif_core.dic 2.0.1*)
Miller index $l$ of the reflection. The values of the Miller indices in the REFLN category must correspond to the cell defined by cell lengths and cell angles in the CELL category.
**[refln]**

`_refln.intensity_calc` (*float*)
`_refln_intensity_calc` (*cif_core.dic 2.0.1*)
The calculated value of the intensity in the same units as `_refln.intensity_meas`.
**[refln]**

`_refln.intensity_meas` (*float*)
`_refln_intensity_meas` (*cif_core.dic 2.0.1*)
The measured value of the intensity.
**[refln]**

`_refln.intensity_sigma` (*float*)
`_refln_intensity_sigma` (*cif_core.dic 2.0.1*)
The standard uncertainty (derived from measurement) of the intensity in the same units as `_refln.intensity_meas`.
**[refln]**

`_refln.mean_path_length_tbar` (*float*)
`_refln_mean_path_length_tbar` (*cif_core.dic 2.3*)
Mean path length in millimetres through the crystal for this reflection.
The permitted range is $[0.0, \infty)$. **[refln]**

`_refln.phase_calc` (*float*)
`_refln_phase_calc` (*cif_core.dic 2.0.1*)
The calculated structure-factor phase in degrees.
**[refln]**

`_refln.phase_meas` (*float*)
`_refln_phase_meas` (*cif_core.dic 2.0.1*)
The measured structure-factor phase in degrees.
**[refln]**

`_refln.refinement_status` (*ucode*)
`_refln_refinement_status` (*cif_core.dic 2.0.1*)
Status of a reflection in the structure-refinement process.
The data value must be one of the following:

| | |
|---|---|
| `incl` | included in least-squares process |
| `excl` | excluded from least-squares process |
| `extn` | excluded due to extinction |

Where no value is given, the assumed value is '`incl`'. **[refln]**

*`_refln.scale_group_code`
`_refln_scale_group_code` (*cif_core.dic 2.0.1*)
This data item is a pointer to `_reflns_scale.group_code` in the REFLNS_SCALE category.

`_refln.sint_over_lambda` (*float*)
`_refln_sint/lambda` (*cif_core.dic 2.0.1*)
The $(\sin\theta)/\lambda$ value in reciprocal ångströms for this reflection.
The permitted range is $[0.0, \infty)$. **[refln]**

`_refln.status` (*ucode*)
`_refln_observed_status` (*cif_core.dic 2.0.1*)
Classification of a reflection so as to indicate its status with respect to inclusion in the refinement and the calculation of $R$ factors.
The data value must be one of the following:

| | |
|---|---|
| `o` | satisfies `_refine.ls_d_res_high`, satisfies `_refine.ls_d_res_low`, observed by `_reflns.observed_criterion`, not flagged as systematically absent, not flagged as unreliable |
| `<` | satisfies `_refine.ls_d_res_high`, satisfies `_refine.ls_d_res_low`, unobserved by `_reflns.observed_criterion`, not flagged as systematically absent, not flagged as unreliable |
| `-` | systematically absent reflection |
| `x` | unreliable measurement – not used |
| `h` | does not satisfy `_refine.ls_d_res_high` |
| `l` | does not satisfy `_refine.ls_d_res_low` |
| `f` | satisfies `_refine.ls_d_res_high`, satisfies `_refine.ls_d_res_low`, observed by `_reflns.observed_criterion`, not flagged as systematically absent, not flagged as unreliable, excluded from refinement so as to be included in the calculation of a 'free' $R$ factor |

**[refln]**

`_refln.symmetry_epsilon` (*int*)
`_refln_symmetry_epsilon` (*cif_core.dic 2.0.1*)
The symmetry reinforcement factor corresponding to the number of times the reflection indices are generated identically from the space-group symmetry operations.
The permitted range is $[1, 48]$. **[refln]**

`_refln.symmetry_multiplicity` (*int*)
`_refln_symmetry_multiplicity` (*cif_core.dic 2.0.1*)
The number of symmetry-equivalent reflections. The equivalent reflections have the same structure-factor magnitudes because of the space-group symmetry and the Friedel relationship.
The permitted range is $[1, 48]$. **[refln]**

`_refln.wavelength` (*float*)
`_refln_wavelength` (*cif_core.dic 2.0.1*)
The mean wavelength in ångströms of radiation used to measure this reflection. This is an important parameter for data collected using energy-dispersive detectors or the Laue method.
The permitted range is $[0.0, \infty)$. **[refln]**

*`_refln.wavelength_id`
`_refln_wavelength_id` (*cif_core.dic 2.0.1*)
This data item is a pointer to `_diffrn_radiation.wavelength_id` in the DIFFRN_RADIATION category.

## REFLN_SYS_ABS

Data items in the REFLN_SYS_ABS category record details about the reflection data that should be systematically absent, given the designated space group.

Category group(s): **inclusive_group**
**refln_group**
Category key(s): **_refln_sys_abs.index_h**
**_refln_sys_abs.index_k**
**_refln_sys_abs.index_l**

*Example 1 – hypothetical example.*

```
loop_
_refln_sys_abs.index_h
_refln_sys_abs.index_k
_refln_sys_abs.index_l
_refln_sys_abs.I
_refln_sys_abs.sigmaI
_refln_sys_abs.I_over_sigmaI
 0  3  0   28.32  22.95  1.23
 0  5  0   14.11  16.38  0.86
 0  7  0  114.81  20.22  5.67
 0  9  0   32.99  24.51  1.35
```

### _refln_sys_abs.I (*float, su*)

*_ebi_refln_sys_abs.I* (*ebi_extensions 1.0*)

The measured value of the intensity in arbitrary units.

Related item: **_refln_sys_abs.sigmaI** (associated esd). **[refln_sys_abs]**

### _refln_sys_abs.I_over_sigmaI (*float*)

*_ebi_refln_sys_abs.I_over_sigma* (*ebi_extensions 1.0*)

The ratio of **_refln_sys_abs.I** to **_refln_sys_abs.sigmaI**. Used to evaluate whether a reflection that should be systematically absent according to the designated space group is in fact absent.

**[refln_sys_abs]**

### *_refln_sys_abs.index_h (*int*)

*_ebi_refln_sys_abs.h* (*ebi_extensions 1.0*)

Miller index *h* of the reflection. The values of the Miller indices in the REFLN_SYS_ABS category must correspond to the cell defined by cell lengths and cell angles in the CELL category.

**[refln_sys_abs]**

### *_refln_sys_abs.index_k (*int*)

*_ebi_refln_sys_abs.k* (*ebi_extensions 1.0*)

Miller index *k* of the reflection. The values of the Miller indices in the REFLN_SYS_ABS category must correspond to the cell defined by cell lengths and cell angles in the CELL category.

**[refln_sys_abs]**

### *_refln_sys_abs.index_l (*int*)

*_ebi_refln_sys_abs.l* (*ebi_extensions 1.0*)

Miller index *l* of the reflection. The values of the Miller indices in the REFLN_SYS_ABS category must correspond to the cell defined by cell lengths and cell angles in the CELL category.

**[refln_sys_abs]**

### _refln_sys_abs.sigmaI (*float*)

*_ebi_refln_sys_abs.sigmaI* (*ebi_extensions 1.0*)

The standard uncertainty (estimated standard deviation) of **_refln_sys_abs.I** in arbitrary units.

Related item: **_refln_sys_abs.I** (associated value). **[refln_sys_abs]**

## REFLNS

Data items in the REFLNS category record details about the reflection data used to determine the ATOM_SITE data items. The REFLN data items refer to individual reflections and must be included in looped lists. The REFLNS data items specify the parameters that apply to all reflections. The REFLNS data items are not looped.

Category group(s): **inclusive_group**
**refln_group**
Category key(s): **_reflns.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_reflns.entry_id                      '5HVP'
_reflns.data_reduction_method
; Xengen program scalei. Anomalous pairs were merged. Scaling
  proceeded in several passes, beginning with 1-parameter
  fit and ending with 3-parameter fit.
;
_reflns.data_reduction_details
; Merging and scaling based on only those reflections
  with I > \s(I).
;

_reflns.d_resolution_high             2.00
_reflns.d_resolution_low              8.00

_reflns.limit_h_max                   22
_reflns.limit_h_min                   0
_reflns.limit_k_max                   46
_reflns.limit_k_min                   0
_reflns.limit_l_max                   57
_reflns.limit_l_min                   0

_reflns.number_obs                    7228
_reflns.observed_criterion            '> 1 \s(I)'
_reflns.details                       none
```

*Example 2 – based on data set TOZ of Willis, Beckwith & Tozer [Acta Cryst. (1991), C**47**, 2276–2277].*

```
_reflns.limit_h_min              0
_reflns.limit_h_max              6
_reflns.limit_k_min              0
_reflns.limit_k_max              17
_reflns.limit_l_min              0
_reflns.limit_l_max              22
_reflns.number_all               1592
_reflns.number_obs               1408
_reflns.observed_criterion       F_>_6.0_\s(F)
_reflns.d_resolution_high        0.8733
_reflns.d_resolution_low         11.9202
```

### _reflns.B_iso_Wilson_estimate (*float*)

The value of the overall isotropic displacement parameter estimated from the slope of the Wilson plot.

**[reflns]**

### _reflns.d_resolution_high (*float*)

*_reflns_d_resolution_high* (*cif_core.dic 2.0.1*)

The smallest value for the interplanar spacings for the reflection data. This is called the highest resolution.

The permitted range is $[0.0, \infty)$. **[reflns]**

### _reflns.d_resolution_low (*float*)

*_reflns_d_resolution_low* (*cif_core.dic 2.0.1*)

The largest value for the interplanar spacings for the reflection data. This is called the lowest resolution.

The permitted range is $[0.0, \infty)$. **[reflns]**

### _reflns.data_reduction_details (*text*)

A description of special aspects of the data-reduction procedures.

Example:

```
; Merging and scaling based on only those
  reflections with I > sig(I).
;
```

**[reflns]**

**_reflns.data_reduction_method** (*text*)

The method used for data reduction. Note that this is not the computer program used, which is described in the SOFTWARE category, but the method itself. This data item should be used to describe significant methodological options used within the data-reduction programs.

Example:

```
; Profile fitting by method of Kabsch (1987).
  Scaling used spherical harmonic coefficients.
;
```

**[reflns]**

**_reflns.details** (*text*)

***_reflns_special_details*** (*cif_core.dic 2.0.1*)

A description of reflection data not covered by other data names. This should include details of the Friedel pairs.

**[reflns]**

* **_reflns.entry_id**

This data item is a pointer to **_entry.id** in the ENTRY category.

**_reflns.Friedel_coverage** (*float*)

***_reflns_Friedel_coverage*** (*cif_core.dic 2.3*)

The proportion of Friedel-related reflections present in the number of 'independent' reflections specified by the item **_reflns.number_all**. This proportion is calculated as the ratio

$$\frac{[N(\text{crystal class}) - N(\text{Laue symmetry})]}{N(\text{Laue symmetry})},$$

where, working from the DIFFRN_REFLN list, $N$(Crystal class) is the number of reflections obtained on averaging under the symmetry of the crystal class and $N$(Laue symmetry) is the number of reflections obtained on averaging under the Laue symmetry.

Examples: (*a*) For centrosymmetric structures, the value of **_reflns.Friedel_coverage** is necessarily equal to 0.0 as the crystal class is identical to the Laue symmetry. (*b*) For whole-sphere data for a crystal in the space group $P1$, **_reflns.Friedel_coverage** is equal to 1.0, as no reflection $hkl$ is equivalent to $-h-k-l$ in the crystal class and all Friedel pairs $\{hkl; -h-k-l\}$ have been measured. (*c*) For whole-sphere data in space group $Pmm2$, **_reflns.Friedel_coverage** will be $< 1.0$ because although reflections $hkl$ and $-h-k-l$ are not equivalent when $hkl$ indices are nonzero, they are when $l = 0$. (*d*) For a crystal in space group $Pmm2$, measurements of the two inequivalent octants $h \geq 0, k \geq 0, l$ lead to the same value as in (*c*), whereas measurements of the two equivalent octants $h \geq 0, k, l \geq 0$ will lead to a value of zero for **_reflns.Friedel_coverage**.

The permitted range is [0.0, 1.0]. **[reflns]**

**_reflns.limit_h_max** (*int*)

***_reflns_limit_h_max*** (*cif_core.dic 2.0.1*)

Maximum value of the Miller index $h$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_h_max**.

**[reflns]**

**_reflns.limit_h_min** (*int*)

***_reflns_limit_h_min*** (*cif_core.dic 2.0.1*)

Minimum value of the Miller index $h$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_h_min**.

**[reflns]**

**_reflns.limit_k_max** (*int*)

***_reflns_limit_k_max*** (*cif_core.dic 2.0.1*)

Maximum value of the Miller index $k$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_k_max**.

**[reflns]**

**_reflns.limit_k_min** (*int*)

***_reflns_limit_k_min*** (*cif_core.dic 2.0.1*)

Minimum value of the Miller index $k$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_k_min**.

**[reflns]**

**_reflns.limit_l_max** (*int*)

***_reflns_limit_l_max*** (*cif_core.dic 2.0.1*)

Maximum value of the Miller index $l$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_l_max**.

**[reflns]**

**_reflns.limit_l_min** (*int*)

***_reflns_limit_l_min*** (*cif_core.dic 2.0.1*)

Minimum value of the Miller index $l$ for the reflection data. This need not have the same value as **_diffrn_reflns.limit_l_min**.

**[reflns]**

**_reflns.number_all** (*int*)

***_reflns_number_total*** (*cif_core.dic 2.0.1*)

The total number of reflections in the REFLN list (not the DIFFRN_REFLN list). This number may contain Friedel-equivalent reflections according to the nature of the structure and the procedures used. The item **_reflns.details** describes the reflection data.

The permitted range is $[0, \infty)$. **[reflns]**

**_reflns.number_gt** (*int*)

***_reflns_number_gt*** (*cif_core.dic 2.3*)

The number of reflections in the REFLN list (not the DIFFRN_REFLN list) that are significantly intense, satisfying the criterion specified by **_reflns.threshold_expression**. This may include Friedel-equivalent reflections (*i.e.* those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class) according to the nature of the structure and the procedures used. Any special characteristics of the reflections included in the REFLN list should be described using the item **_reflns.details**.

The permitted range is $[0, \infty)$. **[reflns]**

**_reflns.number_obs** (*int*)

***_reflns_number_observed*** (*cif_core.dic 2.0.1*)

The number of reflections in the REFLN list (not the DIFFRN_REFLN list) classified as observed (see **_reflns.observed_criterion**). This number may contain Friedel-equivalent reflections according to the nature of the structure and the procedures used.

The permitted range is $[0, \infty)$. **[reflns]**

**_reflns.observed_criterion** (*text*)

***_reflns_observed_criterion*** (*cif_core.dic 2.0.1*)

The criterion used to classify a reflection as 'observed'. This criterion is usually expressed in terms of a $\sigma(I)$ or $\sigma(F)$ threshold.

Related items: **_reflns.observed_criterion_sigma_F** (alternate), **_reflns.observed_criterion_sigma_I** (alternate), **_reflns.observed_criterion_I_min** (alternate), **_reflns.observed_criterion_I_max** (alternate), **_reflns.observed_criterion_F_min** (alternate), **_reflns.observed_criterion_F_max** (alternate) .

Example: '`>2sigma(I)`'. **[reflns]**

**_reflns.observed_criterion_F_max** (*float*)

The criterion used to classify a reflection as 'observed' expressed as an upper limit for the value of $F$.

Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_I_max** (convention). **[reflns]**

**_reflns.observed_criterion_F_min** (*float*)
The criterion used to classify a reflection as 'observed' expressed as a lower limit for the value of $F$.
Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_I_min** (convention). **[reflns]**

**_reflns.observed_criterion_I_max** (*float*)
The criterion used to classify a reflection as 'observed' expressed as an upper limit for the value of $I$.
Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_F_max** (convention). **[reflns]**

**_reflns.observed_criterion_I_min** (*float*)
The criterion used to classify a reflection as 'observed' expressed as a lower limit for the value of $I$.
Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_F_min** (convention). **[reflns]**

**_reflns.observed_criterion_sigma_F** (*float*)
The criterion used to classify a reflection as 'observed' expressed as a multiple of the value of $\sigma(F)$.
Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_sigma_I** (convention). **[reflns]**

**_reflns.observed_criterion_sigma_I** (*float*)
The criterion used to classify a reflection as 'observed' expressed as a multiple of the value of $\sigma(I)$.
Related items: **_reflns.observed_criterion** (alternate), **_reflns.observed_criterion_sigma_F** (convention). **[reflns]**

**_reflns.percent_possible_obs** (*float*)
The percentage of geometrically possible reflections represented by reflections that satisfy the resolution limits established by **_reflns.d_resolution_high** and **_reflns.d_resolution_low** and the observation limit established by **_reflns.observed_criterion**.
The permitted range is $[0.0, \infty)$. **[reflns]**

**_reflns.R_free_details** (*text*)
A description of the method by which a subset of reflections was selected for exclusion from refinement so as to be used in the calculation of a 'free' $R$ factor.
Example:
```
; The data set was sorted with l varying most rapidly and h
varying least rapidly. Every 10th reflection in this sorted
list was excluded from refinement and included in the
calculation of a 'free' R factor.
;
```
**[reflns]**

**_reflns.Rmerge_F_all** (*float*)
Residual factor $R_{\rm merge}$ for all reflections that satisfy the resolution limits established by **_reflns.d_resolution_high** and **_reflns.d_resolution_low**.

$$R_{\rm merge} = \frac{\sum_i(\sum_j |F_j - \langle F\rangle|)}{\sum_i(\sum_j \langle F\rangle)},$$

where $F_j$ = the amplitude of the $j$th observation of reflection $i$, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is $[0.0, \infty)$. **[reflns]**

**_reflns.Rmerge_F_obs** (*float*)
Residual factor $R_{\rm merge}$ for reflections that satisfy the resolution limits established by **_reflns.d_resolution_high** and **_reflns.d_resolution_low** and the observation limit established by **_reflns.observed_criterion**.

$$R_{\rm merge} = \frac{\sum_i(\sum_j |F_j - \langle F\rangle|)}{\sum_i(\sum_j \langle F\rangle)},$$

where $F_j$ = the amplitude of the $j$th observation of reflection $i$, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is $[0.0, \infty)$. **[reflns]**

**_reflns.threshold_expression** (*text*)
***_reflns_threshold_expression*** (*cif_core.dic 2.3*)
The threshold, usually based on multiples of $u(I)$, $u(F^2)$ or $u(F)$, that serves to identify significantly intense reflections, the number of which is given by **_reflns.number_gt**. These reflections are used in the calculation of **_refine.ls_R_factor_gt**.
Related item: **_reflns.observed_criterion** (alternate) .
Example: 'I>2u(I)'. **[reflns]**

## REFLNS_CLASS

Data items in the REFLNS_CLASS category record details of the reflections used to determine the structural parameters for each reflection class.
Category key(s): **_reflns_class.code**

*Example 1 – example corresponding to the one-dimensional incommensurately modulated structure of $K_2SeO_4$.*

```
loop_
 _reflns_class.number_gt
 _reflns_class.code
     584     'Main'
     226     'Sat1'
     50      'Sat2'
```

***_reflns_class.code** (*code*)
***_reflns_class_code*** (*cif_core.dic 2.3*)
The code identifying a certain reflection class.
Examples: '1', 'm1', 's2'. **[reflns_class]**

**_reflns_class.d_res_high** (*float*)
***_reflns_class_d_res_high*** (*cif_core.dic 2.3*)
For each reflection class, the smallest value in ångströms for the interplanar spacings for the reflections used in the refinement. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.d_res_low** (*float*)
***_reflns_class_d_res_low*** (*cif_core.dic 2.3*)
For each reflection class, the largest value in ångströms for the interplanar spacings for the reflections used in the refinement. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.description** (*text*)
***_reflns_class_description*** (*cif_core.dic 2.3*)
Description of each reflection class.
Examples: 'm=1 first order satellites', 'H0L0 common projection reflections'. **[reflns_class]**

**_reflns_class.number_gt** (*int*)
***_reflns_class_number_gt*** (*cif_core.dic 2.3*)
For each reflection class, the number of significantly intense reflections (see **_reflns.threshold_expression**) in the REFLN list (not the DIFFRN_REFLN list). This may include Friedel-equivalent reflections (*i.e.* those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class) according to the nature of the structure and the procedures used. Any special characteristics of the reflections included in the REFLN list should be described using the item **_reflns.details**.
The permitted range is $[0, \infty)$. **[reflns_class]**

**_reflns_class.number_total** (*int*)
***_reflns_class_number_total*** (*cif_core.dic 2.3*)
For each reflection class, the total number of reflections in the REFLN list (not the DIFFRN_REFLN list). This may include Friedel-equivalent reflections (*i.e.* those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class) according to the nature of the structure and the procedures used. Any special characteristics of the reflections included in the REFLN list should be described using the item **_reflns.details**.
The permitted range is $[0, \infty)$. **[reflns_class]**

**_reflns_class.R_factor_all** (*float*)
***_reflns_class_R_factor_all*** (*cif_core.dic 2.3*)
For each reflection class, the residual factor for all reflections included in the refinement. The reflections also satisfy the resolution limits established by **_reflns_class.d_res_high** and **_reflns_class.d_res_low**. This is the conventional *R* factor. See also the definition of **_reflns_class.wR_factor_all**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.R_factor_gt** (*float*)
***_reflns_class_R_factor_gt*** (*cif_core.dic 2.3*)
For each reflection class, the residual factor for significantly intense reflections (see **_reflns.threshold_expression**) included in the refinement. The reflections also satisfy the resolution limits established by **_reflns_class.d_res_high** and **_reflns_class.d_res_low**. This is the conventional *R* factor. See also the definition of **_reflns_class.wR_factor_all**.

$$R = \frac{\sum |F_{\rm obs} - F_{\rm calc}|}{\sum |F_{\rm obs}|},$$

where $F_{\rm obs}$ = the observed structure-factor amplitudes, $F_{\rm calc}$ = the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.R_Fsqd_factor** (*float*)
***_reflns_class_R_Fsqd_factor*** (*cif_core.dic 2.3*)
For each reflection class, the residual factor $R(F^2)$ calculated on the squared amplitudes of the observed and calculated structure factors for the reflections judged significantly intense (*i.e.* satisfying the threshold specified by **_reflns.threshold_expression**) and included in the refinement. The reflections also satisfy the resolution limits established by **_reflns_class.d_res_high** and **_reflns_class.d_res_low**.

$$R(F^2) = \frac{\sum |F^2_{\rm obs} - F^2_{\rm calc}|}{\sum |F^2_{\rm obs}|},$$

where $F^2_{\rm obs}$ = squares of the observed structure-factor amplitudes, $F^2_{\rm calc}$ = squares of the calculated structure-factor amplitudes and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.R_I_factor** (*float*)
***_reflns_class_R_I_factor*** (*cif_core.dic 2.3*)
For each reflection class, the residual factor $R(I)$ for the reflections judged significantly intense (*i.e.* satisfying the threshold specified by **_reflns.threshold_expression**) and included in the refinement. This is most often calculated in Rietveld refinements against powder data, where it is referred to as $R_B$ or $R_{\rm Bragg}$.

$$R(I) = \frac{\sum |I_{\rm obs} - I_{\rm calc}|}{\sum |I_{\rm obs}|},$$

where $I_{\rm obs}$ = the net observed intensities, $I_{\rm calc}$ = the net calculated intensities and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

**_reflns_class.wR_factor_all** (*float*)
***_reflns_class_wR_factor_all*** (*cif_core.dic 2.3*)
For each reflection class, the weighted residual factors for all reflections included in the refinement. The reflections also satisfy the resolution limits established by **_reflns_class.d_res_high** and **_reflns.class_d_res_low**. See also **_reflns_class.R_factor_** definitions.

$$wR = \left( \frac{\sum \left| w|Y_{\rm obs} - Y_{\rm calc}|^2 \right|}{\sum |wY^2_{\rm obs}|} \right)^{1/2},$$

where $Y_{\rm obs}$ = the observed amplitude specified by **_refine.ls_structure_factor_coef**, $Y_{\rm calc}$ = the calculated amplitude specified by **_refine.ls_structure_factor_coef**, $w$ = the least-squares weight and the sum is taken over the reflections of this class.
The permitted range is $[0.0, \infty)$. **[reflns_class]**

## REFLNS_SCALE

Data items in the REFLNS_SCALE category record details about the structure-factor scales. They are referenced from within the REFLN list through **_refln.scale_group_code**.
Category group(s): **inclusive_group**
**refln_group**
Category key(s): **_reflns_scale.group_code**

*Example 1 – based on laboratory records for the collagen-like peptide [(POG)$_4$ EKG (POG)$_5$]$_3$.*

```
_reflns_scale.group_code    SG1
_reflns_scale.meas_F        4.0
```

***_reflns_scale.group_code** (*line*)
***_reflns_scale_group_code*** (*cif_core.dic 2.0.1*)
The code identifying a scale **_reflns_scale.meas_F**, **_reflns_scale.meas_F_squared** or **_reflns_scale.meas_intensity**. These are linked to the REFLN list by the **_refln.scale_group_code**. These codes need not correspond to those in the DIFFRN_SCALE list.
*The following item(s) have an equivalent role in their respective categories:*
***_refln.scale_group_code***.
Examples: '1', '2', 'c1', 'c2'. **[reflns_scale]**

**_reflns_scale.meas_F** (*float*)
***_reflns_scale_meas_F*** (*cif_core.dic 2.0.1*)
A scale associated with **_reflns_scale.group_code**.
The permitted range is $[0.0, \infty)$. **[reflns_scale]**

**_reflns_scale.meas_F_squared** (*float*)
***_reflns_scale_meas_F_squared*** (*cif_core.dic 2.0.1*)
A scale associated with **_reflns_scale.group_code**.
The permitted range is $[0.0, \infty)$. **[reflns_scale]**

**_reflns_scale.meas_intensity** (*float*)
***_reflns_scale_meas_intensity*** (*cif_core.dic 2.0.1*)
A scale associated with **_reflns_scale.group_code**.
The permitted range is $[0.0, \infty)$. **[reflns_scale]**

## REFLNS_SHELL

Data items in the REFLNS_SHELL category record details about the reflection data used to determine the ATOM_SITE data items broken down into shells of resolution.

Category group(s): **inclusive_group**
**refln_group**
Category key(s): **_reflns_shell.d_res_high**
**_reflns_shell.d_res_low**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_reflns_shell.d_res_high
_reflns_shell.d_res_low
_reflns_shell.meanI_over_sigI_obs
_reflns_shell.number_measured_obs
_reflns_shell.number_unique_obs
_reflns_shell.percent_possible_obs
_reflns_shell.Rmerge_F_obs
  31.38  3.82  69.8  9024  2540  96.8   1.98
   3.82  3.03  26.1  7413  2364  95.1   3.85
   3.03  2.65  10.5  5640  2123  86.2   6.37
   2.65  2.41   6.4  4322  1882  76.8   8.01
   2.41  2.23   4.3  3247  1714  70.4   9.86
   2.23  2.10   3.1  1140   812  33.3  13.99
```

***_reflns_shell.d_res_high** (*float*)
***_reflns_shell_d_res_high*** (*cif_core.dic 2.0.1*)
The smallest value in ångströms for the interplanar spacings for the reflections in this shell. This is called the highest resolution.
The permitted range is $[0.0, \infty)$. **[reflns_shell]**

***_reflns_shell.d_res_low** (*float*)
***_reflns_shell_d_res_low*** (*cif_core.dic 2.0.1*)
The highest value in ångströms for the interplanar spacings for the reflections in this shell. This is called the lowest resolution.
The permitted range is $[0.0, \infty)$. **[reflns_shell]**

**_reflns_shell.meanI_over_sigI_all** (*float*)
***_reflns_shell_meanI_over_sigI_all*** (*cif_core.dic 2.0.1*)
The ratio of the mean of the intensities of all reflections in this shell to the mean of the standard uncertainties of the intensities of all reflections in this shell.
**[reflns_shell]**

**_reflns_shell.meanI_over_sigI_gt** (*float*)
***_reflns_shell_meanI_over_sigI_gt*** (*cif_core.dic 2.3*)
The ratio of the mean of the intensities of the significantly intense reflections (see **_reflns.threshold_expression**) in this shell to the mean of the standard uncertainties of the intensities of the significantly intense reflections in this shell.
Related item: **_reflns_shell.meanI_over_uI_gt** (replaces). **[reflns_shell]**

**_reflns_shell.meanI_over_sigI_obs** (*float*)
***_reflns_shell_meanI_over_sigI_obs*** (*cif_core.dic 2.0.1*)
The ratio of the mean of the intensities of the reflections classified as 'observed' (see **_reflns.observed_criterion**) in this shell to the mean of the standard uncertainties of the intensities of the 'observed' reflections in this shell.
**[reflns_shell]**

**_reflns_shell.meanI_over_uI_all** (*float*)
***_reflns_shell_meanI_over_uI_all*** (*cif_core.dic 2.3*)
The ratio of the mean of the intensities of all reflections in this shell to the mean of the standard uncertainties of the intensities of all reflections in this shell.
Related item: **_reflns_shell.meanI_over_sigI_all** (alternate).
**[reflns_shell]**

**_reflns_shell.meanI_over_uI_gt** (*float*)
***_reflns_shell_meanI_over_uI_gt*** (*cif_core.dic 2.3*)
The ratio of the mean of the intensities of the significantly intense reflections (see **_reflns.threshold_expression**) in this shell to the mean of the standard uncertainties of the intensities of the significantly intense reflections in this shell.
Related items: **_reflns_shell.meanI_over_sigI_gt** (alternate), **_reflns_shell.meanI_over_sigI_obs** (alternate). **[reflns_shell]**

**_reflns_shell.number_measured_all** (*int*)
***_reflns_shell_number_measured_all*** (*cif_core.dic 2.0.1*)
The total number of reflections measured for this shell.
**[reflns_shell]**

**_reflns_shell.number_measured_gt** (*int*)
***_reflns_shell_number_measured_gt*** (*cif_core.dic 2.3*)
The number of significantly intense reflections (see **_reflns.threshold_expression**) measured for this shell.
The permitted range is $[0, \infty)$.
Related item: **_reflns_shell.number_measured_obs** (alternate).
**[reflns_shell]**

**_reflns_shell.number_measured_obs** (*int*)
***_reflns_shell_number_measured_obs*** (*cif_core.dic 2.0.1*)
The number of reflections classified as 'observed' (see **_reflns.observed_criterion**) for this shell.
**[reflns_shell]**

**_reflns_shell.number_possible** (*int*)
***_reflns_shell_number_possible*** (*cif_core.dic 2.0.1*)
The number of unique reflections it is possible to measure in this shell.
The permitted range is $[0, \infty)$. **[reflns_shell]**

**_reflns_shell.number_unique_all** (*int*)
***_reflns_shell_number_unique_all*** (*cif_core.dic 2.0.1*)
The total number of measured reflections which are symmetry-unique after merging for this shell.
**[reflns_shell]**

**_reflns_shell.number_unique_gt** (*int*)
***_reflns_shell_number_unique_gt*** (*cif_core.dic 2.3*)
The total number of significantly intense reflections (see **_reflns.threshold_expression**) resulting from merging measured symmetry-equivalent reflections for this resolution shell.
The permitted range is $[0, \infty)$.
Related item: **_reflns_shell.number_unique_obs** (alternate). **[reflns_shell]**

**_reflns_shell.number_unique_obs** (*int*)
***_reflns_shell_number_unique_obs*** (*cif_core.dic 2.0.1*)
The total number of measured reflections classified as 'observed' (see **_reflns.observed_criterion**) which are symmetry-unique after merging for this shell.
**[reflns_shell]**

**_reflns_shell.percent_possible_all** (*float*)
***_reflns_shell_percent_possible_all*** (*cif_core.dic 2.0.1*)
The percentage of geometrically possible reflections represented by all reflections measured for this shell.
The permitted range is [0.0, ∞). **[reflns_shell]**

**_reflns_shell.percent_possible_gt** (*float*)
***_reflns_shell_percent_possible_gt*** (*cif_core.dic 2.3*)
The percentage of geometrically possible reflections represented by significantly intense reflections (see **_reflns.threshold_expression**) measured for this shell.
The permitted range is [0.0, 100.0].
Related item: **_reflns_shell.percent_possible_obs** (alternate).
**[reflns_shell]**

**_reflns_shell.percent_possible_obs** (*float*)
***_reflns_shell_percent_possible_obs*** (*cif_core.dic 2.0.1*)
The percentage of geometrically possible reflections represented by reflections classified as 'observed' (see **_reflns.observed_criterion**) for this shell.
The permitted range is [0.0, ∞). **[reflns_shell]**

**_reflns_shell.Rmerge_F_all** (*float*)
***_reflns_shell_Rmerge_F_all*** (*cif_core.dic 2.0.1*)
Residual factor $R_{\rm merge}$ for all reflections that satisfy the resolution limits established by **_reflns_shell.d_res_high** and **_reflns_shell.d_res_low**.

$$R_{\rm merge} = \frac{\sum_i(\sum_j |F_j - \langle F\rangle|)}{\sum_i(\sum_j \langle F\rangle)},$$

where $F_j$ = the amplitude of the $j$th observation of reflection $i$, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞). **[reflns_shell]**

**_reflns_shell.Rmerge_F_gt** (*float*)
***_reflns_shell_Rmerge_F_gt*** (*cif_core.dic 2.3*)
The value of $R_{\rm merge}(F)$ for significantly intense reflections (see **_reflns.threshold_expression**) in a given shell.

$$R_{\rm merge} = \frac{\sum_i(\sum_j |F_j - \langle F\rangle|)}{\sum_i(\sum_j \langle F\rangle)},$$

where $F_j$ = the amplitude of the $j$th observation of reflection $i$, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞).
Related item: **_reflns_shell.Rmerge_F_obs** (alternate). **[reflns_shell]**

**_reflns_shell.Rmerge_F_obs** (*float*)
***_reflns_shell_Rmerge_F_obs*** (*cif_core.dic 2.0.1*)
Residual factor $R_{\rm merge}$ for reflections that satisfy the resolution limits established by **_reflns_shell.d_res_high** and **_reflns_shell.d_res_low** and the observation criterion established by **_reflns.observed_criterion**.

$$R_{\rm merge} = \frac{\sum_i(\sum_j |F_j - \langle F\rangle|)}{\sum_i(\sum_j \langle F\rangle)},$$

where $F_j$ = the amplitude of the $j$th observation of reflection $i$, $\langle F\rangle$ = the mean of the amplitudes of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞). **[reflns_shell]**

**_reflns_shell.Rmerge_I_all** (*float*)
***_reflns_shell_Rmerge_I_all*** (*cif_core.dic 2.0.1*)
The value of $R_{\rm merge}(I)$ for all reflections in a given shell.

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)},$$

where $I_j$ = the intensity of the $j$th observation of reflection $i$, $\langle I\rangle$ = the mean of the intensities of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞). **[reflns_shell]**

**_reflns_shell.Rmerge_I_gt** (*float*)
***_reflns_shell_Rmerge_I_gt*** (*cif_core.dic 2.3*)
The value of $R_{\rm merge}(I)$ for significantly intense reflections (see **_reflns.threshold_expression**) in a given shell.

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)},$$

where $I_j$ = the intensity of the $j$th observation of reflection $i$, $\langle I\rangle$ = the mean of the intensities of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞).
Related item: **_reflns_shell.Rmerge_I_obs** (alternate). **[reflns_shell]**

**_reflns_shell.Rmerge_I_obs** (*float*)
***_reflns_shell_Rmerge_I_obs*** (*cif_core.dic 2.0.1*)
The value of $R_{\rm merge}(I)$ for reflections classified as 'observed' (see **_reflns.observed_criterion**) in a given shell.

$$R_{\rm merge}(I) = \frac{\sum_i(\sum_j |I_j - \langle I\rangle|)}{\sum_i(\sum_j \langle I\rangle)},$$

where $I_j$ = the intensity of the $j$th observation of reflection $i$, $\langle I\rangle$ = the mean of the intensities of all observations of reflection $i$, $\sum_i$ is taken over all reflections and $\sum_j$ is taken over all observations of each reflection.
The permitted range is [0.0, ∞). **[reflns_shell]**

## SOFTWARE

Data items in the SOFTWARE category record details about the software used in the structure analysis, which implies any software used in the generation of any data items associated with the structure determination and structure representation. These data items allow computer programs to be referenced in more detail than data items in the COMPUTING category do.

Category group(s): **inclusive_group**
**computing_group**
Category key(s): **_software.name**
**_software.version**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_software.name
_software.version
_software.date
_software.type
_software.contact_author
_software.contact_author_email
_software.location
_software.classification
_software.citation_id
_software.language
_software.compiler_name
_software.compiler_version
_software.hardware
_software.os
_software.os_version
_software.dependencies
_software.mods
_software.description
   Prolsq   unknown  .   program   'Wayne A. Hendrickson'  ?
   'ftp://rosebud.sdsc.edu/pub/sdsc/xtal/CCP4/ccp4/'
   refinement ref5  Fortran
   'Convex Fortran' v8.0 'Convex C220' ConvexOS  v10.1
   'Requires that Protin be run first'    optimized
   'restrained least-squares refinement'
```

**_software.citation_id**
This data item is a pointer to **_citation.id** in the CITATION category.

**_software.classification** (*uline*)
The classification of the program according to its major function.
Examples: 'data collection', 'data reduction', 'phasing', 'model building', 'refinement', 'validation', 'other'. **[software]**

**_software.compiler_name** (*line*)
The compiler used to compile the software.
Examples: 'Convex Fortran', 'gcc', 'DEC C'. **[software]**

**_software.compiler_version** (*line*)
The version of the compiler used to compile the software.
Examples: '3.1', '2.1 alpha'. **[software]**

**_software.contact_author** (*line*)
The recognized contact author of the software. This could be the original author, someone who has modified the code or someone who maintains the code. It should be the person most commonly associated with the code.
Examples: 'T. Alwyn Jones', 'Axel Brunger'. **[software]**

**_software.contact_author_email** (*line*)
The e-mail address of the person specified in **_software.contact_author**.
Example: 'bourne@sdsc.edu'. **[software]**

**_software.date** (*line*)
The date the software was released.
Examples: '1991-10-01', '1990-04-30'. **[software]**

**_software.dependencies** (*line*)
Any prerequisite software required to run **_software.name**.
Example: 'PDBlib class library'. **[software]**

**_software.description** (*line*)
Description of the software.
Example: 'Uses method of restrained least squares'. **[software]**

**_software.hardware** (*line*)
The hardware upon which the software was run.
Examples: 'Sun Sparc 10 model 41', 'Dec Alpha 3000 model 500S', 'Silicon Graphics Elan', 'Compaq PC 486/66'. **[software]**

**_software.language** (*uline*)
The major computing language in which the software is coded.
The data value must be one of the following:
Ada
assembler
Awk
Basic
C++
C/C++
C
csh
Fortran
Fortran_77
'Fortran 77'
'Fortran 90'
Java
ksh
Pascal
Perl
Python
sh
Tcl
Other **[software]**

**_software.location** (*line*)
The URL for an Internet address at which details of the software can be found.
Examples:
'http://rosebud.sdsc.edu/projects/pb/IUCr/software.html',
'ftp://ftp.sdsc.edu/pub/sdsc/biology/'. **[software]**

**_software.mods** (*line*)
Any noteworthy modifications to the base software, if applicable.
Example: 'Added support for space group F432'. **[software]**

* **_software.name** (*text*)
The name of the software.
Examples: 'Merlot', 'O', 'Xengen', 'X-plor'. **[software]**

**_software.os** (*text*)
The name of the operating system under which the software runs.
Examples: 'Ultrix', 'OpenVMS', 'DOS', 'Windows 95', 'Windows NT', 'Irix', 'HPUX', 'DEC Unix'. **[software]**

**_software.os_version** (*text*)
The version of the operating system under which the software runs.
Examples: '3.1', '4.2.1'. **[software]**

**_software.type** (*uline*)

The classification of the software according to the most common types.

The data value must be one of the following:

| | |
|---|---|
| program | individual program with limited functionality |
| library | used by a program at load time |
| package | collections of programs with multiple functionality |
| filter | filters input and output streams |
| jiffy | short, simple program |
| other | all other kinds of software |

**[software]**

***_software.version** (*line*)

The version of the software.

Examples: 'v1.0', 'beta', '3.1-2', 'unknown'. **[software]**

## SPACE_GROUP

Contains all the data items that refer to the space group as a whole, such as its name or crystal system. They may be looped, for example, in a list of space groups and their properties. Only a subset of the SPACE_GROUP category items appear in this dictionary. The remainder are found in the symmetry CIF dictionary. Space-group types are identified by their number as given in *International Tables for Crystallography* Vol. A. Specific settings of the space groups can be identified either by their Hall symbol or by specifying their symmetry operations. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but several different Hermann–Mauguin symbols may refer to the same space-group type. A Hermann–Mauguin symbol contains information on the choice of the basis, but not on the choice of origin. Different formats for the Hermann–Mauguin symbol are found in the symmetry CIF dictionary.

Category key(s): **_space_group.id**

*Example 1 – the monoclinic space group No. 15 with unique axis b.*

```
_space_group.id                 1
_space_group.name_H-M_alt       'C 2/c'
_space_group.IT_number          15
_space_group.name_Hall          '-C 2yc'
_space_group.crystal_system     monoclinic
```

**_space_group.crystal_system** (*code*)

***_space_group_crystal_system*** (*cif_core.dic 2.3*)

The name of the system of geometric crystal classes of space groups (crystal system) to which the space group belongs. Note that rhombohedral space groups belong to the trigonal system.

Related item: **_symmetry.cell_setting** (alternate).

The data value must be one of the following:

triclinic
monoclinic
orthorhombic
tetragonal
trigonal
hexagonal
cubic

**[space_group]**

***_space_group.id** (*code*)

***_space_group_id*** (*cif_core.dic 2.3*)

This is the unique identifier for the SPACE_GROUP category.

**[space_group]**

**_space_group.IT_number** (*int*)

***_space_group_IT_number*** (*cif_core.dic 2.3*)

The number as assigned in *International Tables for Crystallography* Vol. A, specifying the proper affine class (*i.e.* the orientation-preserving affine class) of space groups (crystallographic space-group type) to which the space group belongs. This number defines the space-group type but not the coordinate system in which it is expressed.

The permitted range is [1, 230].

Related item: **_symmetry.Int_Tables_number** (alternate). **[space_group]**

**_space_group.name_H-M_alt** (*line*)

***_space_group_name_H-M_alt*** (*cif_core.dic 2.3*)

**_space_group.name_H-M_alt** allows any Hermann–Mauguin symbol to be given. The way in which this item is used is determined by the user and in general is not intended to be interpreted by computer. It may, for example, be used to give one of the extended Hermann–Mauguin symbols given in Table 4.3.2.1 of *International Tables for Crystallography* Vol. A (2002) or a Hermann–Mauguin symbol for a conventional or unconventional setting. Each component of the space-group name is separated by a space or an underscore. The use of a space is strongly recommended. The underscore is only retained because it was used in old CIFs. It should not be used in new CIFs. Subscripts should appear without special symbols. Bars should be given as negative signs before the numbers to which they apply. The commonly used Hermann–Mauguin symbol determines the space-group type uniquely but a given space-group type may be described by more than one Hermann–Mauguin symbol. The space-group type is best described using **_space_group.IT_number**. The Hermann–Mauguin symbol may contain information on the choice of basis, but not on the choice of origin. To define the setting uniquely, use **_space_group.name_Hall** or list the symmetry operations.

Related item: **_symmetry.space_group_name_H-M** (alternate) .

Example:

```
; loop_
  _space_group.name_H-M_alt
  'C m c m'
  'C 2/c 2/m 21/m'
  'A m a m'
;  (three examples for space group No. 63)
```

**[space_group]**

**_space_group.name_Hall** (*line*)

***_space_group_name_Hall*** (*cif_core.dic 2.3*)

Space-group symbol defined by Hall. Each component of the space-group name is separated by a space or an underscore. The use of a space is strongly recommended. The underscore is only retained because it was used in old CIFs. It should not be used in new CIFs. **_space_group.name_Hall** uniquely defines the space group and its reference to a particular coordinate system.

Reference: Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525; erratum (1981), A**37**, 921. [See also *International Tables for Crystallography* Vol. B (2001), Chapter 1.4, Appendix 1.4.2.]

Related item: **_symmetry.space_group_name_Hall** (alternate) .

Examples: '`P 2c -2ac`' (equivalent to $Pca2_1$), '`-I 4bd 2ab 3`' (equivalent to $Ia\bar{3}d$).

**[space_group]**

## SPACE_GROUP_SYMOP

Contains information about the symmetry operations of the space group.

Category key(s): **_space_group_symop.id**

*Example 1 – The symmetry operations for the space group $P2_1/c$.*

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
  1    x,y,z
  2   -x,-y,-z
  3   -x,1/2+y,1/2-z
  4    x,1/2-y,1/2+z
```

### *_space_group_symop.id (*code*)

***_space_group_symop_id*** (*cif_core.dic 2.3*)

An arbitrary identifier that uniquely labels each symmetry operation in the list.

Related item: **_symmetry_equiv.id** (alternate). **[space_group_symop]**

### _space_group_symop.operation_xyz (*line*)

***_space_group_symop_operation_xyz*** (*cif_core.dic 2.3*)

A parsable string giving one of the symmetry operations of the space group in algebraic form. If $W$ is a matrix representation of the rotational part of the symmetry operation defined by the positions and signs of $x$, $y$ and $z$, and $\mathbf{w}$ is a column of translations defined by fractions, an equivalent position $\boldsymbol{x}'$ is generated from a given position $\boldsymbol{x}$ by

$$\boldsymbol{x}' = W\boldsymbol{x} + \mathbf{w}.$$

When a list of symmetry operations is given, it must contain a complete set of coordinate representatives which generates all the operations of the space group by the addition of all primitive translations of the space group. Such representatives are to be found as the coordinates of the general-equivalent position in *International Tables for Crystallography* Vol. A (2002), to which it is necessary to add any centring translations shown above the general-equivalent position. That is to say, it is necessary to list explicitly all the symmetry operations required to generate all the atoms in the unit cell defined by the setting used.

Related item: **_symmetry_equiv.pos_as_xyz** (alternate) .

Example: '`x,1/2-y,1/2+z`' (glide reflection through the plane ($x$, 1/4, $z$), with glide vector (1/2)**c**). **[space_group_symop]**

### _space_group_symop.sg_id (*code*)

***_space_group_symop_sg_id*** (*cif_core.dic 2.3*)

This must match a particular value of **_space_group.id**, allowing the symmetry operation to be identified with a particular space group.

**[space_group_symop]**

## STRUCT

Data items in the STRUCT category record details about the description of the crystallographic structure.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_struct.entry_id                    '5HVP'
_struct.title
; HIV-1 protease complex with acetyl-pepstatin
;
```

### *_struct.entry_id

This data item is a pointer to **_entry.id** in the ENTRY category.

### _struct.title (*text*)

A title for the data block. The author should attempt to convey the essence of the structure archived in the CIF in the title, and to distinguish this structural result from others.

Examples: '`5'-D(*(I)CP*CP*GP*G)-3`', '`T4 lysozyme mutant - S32A`', '`hen egg white lysozyme at -30 degrees C`', '`quail egg white lysozyme at 2 atmospheres`'. **[struct]**

## STRUCT_ASYM

Data items in the STRUCT_ASYM category record details about the structural elements in the asymmetric unit.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct_asym.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_asym.id
_struct_asym.entity_id
_struct_asym.details
  A  1  'one monomer of the dimeric enzyme'
  B  1  'one monomer of the dimeric enzyme'
  C  2  'one partially occupied position for the inhibitor'
  D  2  'one partially occupied position for the inhibitor'
```

### _struct_asym.details (*text*)

A description of special aspects of this portion of the contents of the asymmetric unit.

Example:

```
; The drug binds to this enzyme in two roughly twofold
symmetric modes. Hence this biological unit (3) is roughly
twofold symmetric to biological unit (2). Disorder in the
protein chain indicated with alternative ID 2 should be used
with this biological unit.
;
```

**[struct_asym]**

### *_struct_asym.entity_id

This data item is a pointer to **_entity.id** in the ENTITY category.

### *_struct_asym.id (*code*)

The value of **_struct_asym.id** must uniquely identify a record in the STRUCT_ASYM list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_atom_site.label_asym_id***,
***_struct_biol_gen.asym_id***,
***_geom_angle.atom_site_label_asym_id_1***,
***_geom_angle.atom_site_label_asym_id_2***,
***_geom_angle.atom_site_label_asym_id_3***,
***_geom_bond.atom_site_label_asym_id_1***,
***_geom_bond.atom_site_label_asym_id_2***,
***_geom_contact.atom_site_label_asym_id_1***,
***_geom_contact.atom_site_label_asym_id_2***,
***_geom_hbond.atom_site_label_asym_id_A***,
***_geom_hbond.atom_site_label_asym_id_D***,
***_geom_hbond.atom_site_label_asym_id_H***,
***_geom_torsion.atom_site_label_asym_id_1***,
***_geom_torsion.atom_site_label_asym_id_2***,
***_geom_torsion.atom_site_label_asym_id_3***,
***_geom_torsion.atom_site_label_asym_id_4***,
***_struct_conf.beg_label_asym_id***,
***_struct_conf.end_label_asym_id***,
***_struct_conn.ptnr1_label_asym_id***,

***_struct_conn.ptnr2_label_asym_id***,
***_struct_mon_nucl.label_asym_id***,
***_struct_mon_prot.label_asym_id***,
***_struct_mon_prot_cis.label_asym_id***,
***_struct_ncs_dom_lim.beg_label_asym_id***,
***_struct_ncs_dom_lim.end_label_asym_id***,
***_struct_sheet_range.beg_label_asym_id***,
***_struct_sheet_range.end_label_asym_id***,
***_struct_site_gen.label_asym_id***.
Examples: '1', 'A', '2B3'. **[struct_asym]**

## STRUCT_BIOL

Data items in the STRUCT_BIOL category record details about the structural elements that form each structure of biological significance. A given crystal structure may contain many different biological structures. A given structural component in the asymmetric unit may be part of more than one biological unit. A given biological structure may involve crystallographic symmetry. For instance, in a structure of a lysozyme–FAB structure, the light- and heavy-chain components of the FAB could be one biological unit, while the two chains of the FAB and the lysozyme could constitute a second biological unit.
Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_biol.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_biol.id
_struct_biol.details
  1
; significant deviations from twofold symmetry exist in this
  dimeric enzyme
;
  2
; The drug binds to this enzyme in two roughly twofold
  symmetric modes. Hence this biological unit (2) is roughly
  twofold symmetric to biological unit (3). Disorder in the
  protein chain indicated with alternative ID 1 should be
  used with this biological unit.
;
  3
; The drug binds to this enzyme in two roughly twofold
  symmetric modes. Hence this biological unit (3) is roughly
  twofold symmetric to biological unit (2). Disorder in the
  protein chain indicated with alternative ID 2 should be
  used with this biological unit.
;
```

### **_struct_biol.details** (*text*)

A description of special aspects of the biological unit.
Example:
```
; The drug binds to this enzyme in two roughly twofold
symmetric modes. Hence this biological unit (3) is roughly
twofold symmetric to biological unit (2). Disorder in the
protein chain indicated with alternative ID 2 should be used
with this biological unit.
;
```
**[struct_biol]**

### * **_struct_biol.id** (*line*)

The value of **_struct_biol.id** must uniquely identify a record in the STRUCT_BIOL list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_struct_biol_gen.biol_id***,
***_struct_biol_keywords.biol_id***,
***_struct_biol_view.biol_id***,
***_struct_ref.biol_id***. **[struct_biol]**

## STRUCT_BIOL_GEN

Data items in the STRUCT_BIOL_GEN category record details about the generation of each biological unit. The STRUCT_BIOL_GEN data items provide the specifications of the components that constitute that biological unit, which may include symmetry elements.
Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_biol_gen.biol_id**
**_struct_biol_gen.asym_id**
**_struct_biol_gen.symmetry**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_biol_gen.biol_id
_struct_biol_gen.asym_id
_struct_biol_gen.symmetry
  1  A  1_555
  1  B  1_555
  2  A  1_555
  2  B  1_555
  2  C  1_555
  3  A  1_555
  3  B  1_555
  3  D  1_555
```

### * **_struct_biol_gen.asym_id**

This data item is a pointer to **_struct_asym.id** in the STRUCT_ASYM category.

### * **_struct_biol_gen.biol_id**

This data item is a pointer to **_struct_biol.id** in the STRUCT_BIOL category.

### **_struct_biol_gen.details** (*text*)

A description of special aspects of the symmetry generation of this portion of the biological structure.
Example:
```
; The zinc atom lies on a special position; application of
symmetry elements to generate the insulin hexamer will
generate excess zinc atoms, which must be removed by hand.
;
```
**[struct_biol_gen]**

### * **_struct_biol_gen.symmetry** (*symop*)

Describes the symmetry operation that should be applied to the atom set specified by **_struct_biol_gen.asym_id** to generate a portion of the biological structure.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[struct_biol_gen]**

## STRUCT_BIOL_KEYWORDS

Data items in the STRUCT_BIOL_KEYWORDS category record keywords that describe each biological unit.
Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_biol_keywords.biol_id**
**_struct_biol_keywords.text**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_biol_keywords.biol_id
_struct_biol_keywords.text
  1  'aspartyl-protease'
  1  'aspartic-protease'
  1  'acid-protease'
  1  'aspartyl-proteinase'
  1  'aspartic-proteinase'
  1  'acid-proteinase'
  1  'enzyme'
  1  'protease'
  1  'proteinase'
  1  'dimer'
  2  'drug-enzyme complex'
  2  'inhibitor-enzyme complex'
  2  'drug-protease complex'
  2  'inhibitor-protease complex'
  3  'drug-enzyme complex'
  3  'inhibitor-enzyme complex'
  3  'drug-protease complex'
  3  'inhibitor-protease complex'
```

* **_struct_biol_keywords.biol_id**

This data item is a pointer to **_struct_biol.id** in the STRUCT_BIOL category.

* **_struct_biol_keywords.text** (*text*)

Keywords describing this biological entity.

Examples: 'antibody', 'antigen', 'enzyme', 'cytokine', 'tRNA'.

**[struct_biol_keywords]**

## STRUCT_BIOL_VIEW

Data items in the STRUCT_BIOL_VIEW category record details about how to draw and annotate an informative view of the biological structure.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct_biol_view.biol_id**
**_struct_biol_view.id**

*Example 1 – based on NDB structure GDL001 by Coll, Aymami, Van Der Marel, Van Boom, Rich & Wang [Biochemistry, (1989), **28**, 310–320].*

```
_struct_biol_view.biol_id              c1
_struct_biol_view.id                   1
_struct_biol_view.rot_matrix[1][1]     0.132
_struct_biol_view.rot_matrix[1][2]     0.922
_struct_biol_view.rot_matrix[1][3]    -0.363
_struct_biol_view.rot_matrix[2][1]     0.131
_struct_biol_view.rot_matrix[2][2]    -0.380
_struct_biol_view.rot_matrix[2][3]    -0.916
_struct_biol_view.rot_matrix[3][1]    -0.982
_struct_biol_view.rot_matrix[3][2]     0.073
_struct_biol_view.rot_matrix[3][3]    -0.172
_struct_biol_view.details
; This view highlights the ATAT-Netropsin interaction in the
  DNA-drug complex.
;
```

* **_struct_biol_view.biol_id**

This data item is a pointer to **_struct_biol.id** in the STRUCT_BIOL category.

**_struct_biol_view.details** (*text*)

A description of special aspects of this view of the biological structure. This data item can be used as a figure legend.

Example:

```
; The enzyme has been oriented with the molecular twofold axis
aligned with the horizontal axis of the figure.
;
```

**[struct_biol_view]**

* **_struct_biol_view.id** (*line*)

The value of **_struct_biol_view.id** must uniquely identify a record in the STRUCT_BIOL_VIEW list. Note that this item need not be a number; it can be any unique identifier.

Examples: 'Figure 1', 'unliganded enzyme', 'view down enzyme active site'.

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[1][1]** (*float*)

The [1][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[1][2]** (*float*)

The [1][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[1][3]** (*float*)

The [1][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}}$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[2][1]** (*float*)

The [2][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[2][2]** (*float*)
The [2][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[2][3]** (*float*)
The [2][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[3][1]** (*float*)
The [3][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[3][2]** (*float*)
The [3][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

**_struct_biol_view.rot_matrix[3][3]** (*float*)
The [3][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_BIOL_GEN category to give a view useful for describing the structure. The conventions used in the rotation are described in **_struct_biol_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_biol_view]**

## STRUCT_CONF

Data items in the STRUCT_CONF category record details about the backbone conformation of a segment of polymer. Data items in the STRUCT_CONF_TYPE category define the criteria used to identify the backbone conformations.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_conf.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_conf.id
_struct_conf.conf_type_id
_struct_conf.beg_label_comp_id
_struct_conf.beg_label_asym_id
_struct_conf.beg_label_seq_id
_struct_conf.end_label_comp_id
_struct_conf.end_label_asym_id
_struct_conf.end_label_seq_id
_struct_conf.details
  HELX1  HELX_RH_AL_P  ARG  A   87  GLN  A   92  .
  HELX2  HELX_RH_AL_P  ARG  B  287  GLN  B  292  .
  STRN1  STRN          PRO  A    1  LEU  A    5  .
  STRN2  STRN          CYS  B  295  PHE  B  299  .
  STRN3  STRN          CYS  A   95  PHE  A  299  .
  STRN4  STRN          PRO  B  201  LEU  B  205  .
# - - - - data truncated for brevity - - - -
  TURN1  TURN_TY1P_P   ILE  A   15  GLN  A   18  .
  TURN2  TURN_TY2_P    GLY  A   49  GLY  A   52  .
  TURN3  TURN_TY1P_P   ILE  A   55  HIS  A   69  .
  TURN4  TURN_TY1_P    THR  A   91  GLY  A   94  .
# - - - - data truncated for brevity - - - -
```

**_struct_conf.beg_auth_asym_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_conf.beg_auth_comp_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_conf.beg_auth_seq_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

***_struct_conf.beg_label_asym_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_conf.beg_label_comp_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_conf.beg_label_seq_id**
A component of the identifier for the residue at which the conformation segment begins. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

***_struct_conf.conf_type_id**
This data item is a pointer to **_struct_conf_type.id** in the STRUCT_CONF_TYPE category.

**_struct_conf.details** (*text*)
A description of special aspects of the conformation assignment.

**[struct_conf]**

**_struct_conf.end_auth_asym_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_conf.end_auth_comp_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_conf.end_auth_seq_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

***_struct_conf.end_label_asym_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_conf.end_label_comp_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_conf.end_label_seq_id**
A component of the identifier for the residue at which the conformation segment ends. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

***_struct_conf.id** (*code*)
The value of **_struct_conf.id** must uniquely identify a record in the STRUCT_CONF list. Note that this item need not be a number; it can be any unique identifier.

**[struct_conf]**

## STRUCT_CONF_TYPE

Data items in the STRUCT_CONF_TYPE category record details about the criteria used to identify backbone conformations of a segment of polymer.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_conf_type.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_conf_type.id
_struct_conf_type.criteria
_struct_conf_type.reference
  HELX_RH_AL_P  'author judgement'  .
  STRN          'author judgement'  .
  TURN_TY1_P    'author judgement'  .
  TURN_TY1P_P   'author judgement'  .
  TURN_TY2_P    'author judgement'  .
  TURN_TY2P_P   'author judgement'  .
```

***_struct_conf_type.id** (*ucode*)
The descriptor that categorizes the type of the conformation of the backbone of the polymer (whether protein or nucleic acid). Explicit values for the torsion angles that define each conformation are not given here, but it is expected that the author would provide such information in either the **_struct_conf_type.criteria** or **_struct_conf_type.reference** data items, or both.

*The following item(s) have an equivalent role in their respective categories:*
***_struct_conf.conf_type_id***.

The data value must be one of the following:

| | |
|---|---|
| HELX_P | helix with handedness and type not specified (protein) |
| HELX_OT_P | helix with handedness and type that do not conform to an accepted category (protein) |
| HELX_RH_P | right-handed helix with type not specified (protein) |
| HELX_RH_OT_P | right-handed helix with type that does not conform to an accepted category (protein) |
| HELX_RH_AL_P | right-handed $\alpha$ helix (protein) |
| HELX_RH_GA_P | right-handed $\gamma$ helix (protein) |
| HELX_RH_OM_P | right-handed $\omega$ helix (protein) |
| HELX_RH_PI_P | right-handed $\pi$ helix (protein) |
| HELX_RH_27_P | right-handed 2–7 helix (protein) |
| HELX_RH_3T_P | right-handed 3–10 helix (protein) |
| HELX_RH_PP_P | right-handed polyproline helix (protein) |
| HELX_LH_P | left-handed helix with type not specified (protein) |
| HELX_LH_OT_P | left-handed helix with type that does not conform to an accepted category (protein) |
| HELX_LH_AL_P | left-handed $\alpha$ helix (protein) |
| HELX_LH_GA_P | left-handed $\gamma$ helix (protein) |
| HELX_LH_OM_P | left-handed $\omega$ helix (protein) |
| HELX_LH_PI_P | left-handed $\pi$ helix (protein) |
| HELX_LH_27_P | left-handed 2–7 helix (protein) |
| HELX_LH_3T_P | left-handed 3–10 helix (protein) |
| HELX_LH_PP_P | left-handed polyproline helix (protein) |
| HELX_N | helix with handedness and type not specified (nucleic acid) |
| HELX_OT_N | helix with handedness and type that do not conform to an accepted category (nucleic acid) |
| HELX_RH_N | right-handed helix with type not specified (nucleic acid) |
| HELX_RH_OT_N | right-handed helix with type that does not conform to an accepted category (nucleic acid) |
| HELX_RH_A_N | right-handed A helix (nucleic acid) |
| HELX_RH_B_N | right-handed B helix (nucleic acid) |
| HELX_RH_Z_N | right-handed Z helix (nucleic acid) |
| HELX_LH_N | left-handed helix with type not specified (nucleic acid) |
| HELX_LH_OT_N | left-handed helix with type that does not conform to an accepted category (nucleic acid) |
| HELX_LH_A_N | left-handed A helix (nucleic acid) |
| HELX_LH_B_N | left-handed B helix (nucleic acid) |
| HELX_LH_Z_N | left-handed Z helix (nucleic acid) |
| TURN_P | turn with type not specified (protein) |
| TURN_OT_P | turn with type that does not conform to an accepted category (protein) |
| TURN_TY1_P | type I turn (protein) |
| TURN_TY1P_P | type I′ turn (protein) |
| TURN_TY2_P | type II turn (protein) |
| TURN_TY2P_P | type II′ turn (protein) |
| TURN_TY3_P | type III turn (protein) |
| TURN_TY3P_P | type III′ turn (protein) |
| STRN | $\beta$ strand (protein) |

**[struct_conf_type]**

**_struct_conf_type.criteria** (*text*)
The criteria used to assign this conformation type.

Examples: 'author judgement', 'phi=54-74, psi=30-50'.

**[struct_conf_type]**

**_struct_conf_type.reference** (*text*)
A literature reference that defines the criteria used to assign this conformation type and subtype.

**[struct_conf_type]**

## STRUCT_CONN

Data items in the STRUCT_CONN category record details about the connections between portions of the structure. These can be hydrogen bonds, salt bridges, disulfide bridges and so on. The STRUCT_CONN_TYPE records define the criteria used to identify these connections.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_conn.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_conn.id
_struct_conn.conn_type_id
_struct_conn.ptnr1_label_comp_id
_struct_conn.ptnr1_label_asym_id
_struct_conn.ptnr1_label_seq_id
_struct_conn.ptnr1_label_atom_id
_struct_conn.ptnr1_role
_struct_conn.ptnr1_symmetry
_struct_conn.ptnr2_label_comp_id
_struct_conn.ptnr2_label_asym_id
_struct_conn.ptnr2_label_seq_id
_struct_conn.ptnr2_label_atom_id
_struct_conn.ptnr2_role
_struct_conn.ptnr2_symmetry
_struct_conn.details
C1  saltbr  ARG  A  87 NZ1 positive 1_555 GLU  A  92  OE1
     negative 1_555  .
C2  hydrog  ARG  B 287 N   donor    1_555 GLY  B 292  O
     acceptor 1_555  .
# - - - - data truncated for brevity - - - -
```

***_struct_conn.conn_type_id**
This data item is a pointer to **_struct_conn_type.id** in the STRUCT_CONN_TYPE category.

**_struct_conn.details** (*text*)
A description of special aspects of the connection.
Example: 'disulfide bridge C-S-S-C is highly distorted'.
**[struct_conn]**

***_struct_conn.id** (*code*)
The value of **_struct_conn.id** must uniquely identify a record in the STRUCT_CONN list. Note that this item need not be a number; it can be any unique identifier.
**[struct_conn]**

**_struct_conn.ptnr1_auth_asym_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_conn.ptnr1_auth_atom_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_conn.ptnr1_auth_comp_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_conn.ptnr1_auth_seq_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_struct_conn.ptnr1_label_alt_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_struct_conn.ptnr1_label_asym_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_conn.ptnr1_label_atom_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_struct_conn.ptnr1_label_comp_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_conn.ptnr1_label_seq_id**
A component of the identifier for partner 1 of the structure connection. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_conn.ptnr1_role** (*uline*)
The chemical or structural role of the first partner in the structure connection.
Examples: 'donor', 'acceptor', 'negative', 'positive', 'metal', 'metal coordination'. **[struct_conn]**

**_struct_conn.ptnr1_symmetry** (*symop*)
Describes the symmetry operation that should be applied to the atom set specified by **_struct_conn.ptnr1_label*** to generate the first partner in the structure connection.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[struct_conn]**

**_struct_conn.ptnr2_auth_asym_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_conn.ptnr2_auth_atom_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_conn.ptnr2_auth_comp_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_conn.ptnr2_auth_seq_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_struct_conn.ptnr2_label_alt_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_struct_conn.ptnr2_label_asym_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_conn.ptnr2_label_atom_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_struct_conn.ptnr2_label_comp_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_conn.ptnr2_label_seq_id**
A component of the identifier for partner 2 of the structure connection. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_conn.ptnr2_role** (*uline*)
The chemical or structural role of the second partner in the structure connection.
Examples: 'donor', 'acceptor', 'negative', 'positive', 'metal', 'metal coordination'. **[struct_conn]**

**_struct_conn.ptnr2_symmetry** (*symop*)
Describes the symmetry operation that should be applied to the atom set specified by **_struct_conn.ptnr2_label*** to generate the second partner in the structure connection.
Examples: '.' (no symmetry or translation to site), '4' (4th symmetry operation applied), '7_645' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[struct_conn]**

## STRUCT_CONN_TYPE

Data items in the STRUCT_CONN_TYPE category record details about the criteria used to identify interactions between portions of the structure.
Category group(s): **inclusive_group**, **struct_group**
Category key(s): **_struct_conn_type.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_conn_type.id
_struct_conn_type.criteria
_struct_conn_type.reference
  saltbr
 'negative to positive distance > 2.5 \%A, < 3.2 \%A'      .
  hydrog
 'NO distance > 2.5\%A, < 3.5\%A, NOC angle < 120 degrees' .
```

**_struct_conn_type.criteria** (*text*)
The criteria used to define the interaction.
Examples: 'O to N distance > 2.5 \%A, < 3.2 \%A', 'authors judgement'. **[struct_conn_type]**

***_struct_conn_type.id** (*ucode*)
The chemical or structural type of the interaction.
*The following item(s) have an equivalent role in their respective categories:* ***_struct_conn.conn_type_id***.
The data value must be one of the following:

| | |
|---|---|
| covale | covalent bond |
| disulf | disulfide bridge |
| hydrog | hydrogen bond |
| metalc | metal coordination |
| mismat | mismatched base pairs |
| saltbr | ionic interaction |
| modres | covalent residue modification |
| covale_base | covalent modification of a nucleotide base |
| covale_sugar | covalent modification of a nucleotide sugar |
| covale_phosphate | covalent modification of a nucleotide phosphate |

**[struct_conn_type]**

**_struct_conn_type.reference** (*text*)
A reference that specifies the criteria used to define the interaction. **[struct_conn_type]**

## STRUCT_KEYWORDS

Data items in the STRUCT_KEYWORDS category specify keywords that describe the chemical structure in this entry.
Category group(s): **inclusive_group**, **struct_group**
Category key(s): **_struct_keywords.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_keywords.entry_id
_struct_keywords.text
 '5HVP' 'enzyme-inhibitor complex'
 '5HVP' 'aspartyl protease'
 '5HVP' 'structure-based drug design'
 '5HVP' 'static disorder'
```

***_struct_keywords.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_struct_keywords.text** (*text*)
Keywords describing this structure.
Examples: 'serine protease', 'inhibited complex', 'high-resolution refinement'. **[struct_keywords]**

## STRUCT_MON_DETAILS

Data items in the STRUCT_MON_DETAILS category record details about specifics of calculations summarized in data items in the STRUCT_MON_PROT and STRUCT_MON_NUCL categories. These can include the coefficients used in map calculations, the radii used for including points in a calculation and so on.
Category group(s): **inclusive_group**, **struct_group**
Category key(s): **_struct_mon_details.entry_id**

***_struct_mon_details.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_struct_mon_details.prot_cis** (*float*)
An ideal *cis* peptide bond would have an $\omega$ torsion angle of zero. This data item gives the value in degrees by which the observed torsion angle can differ from 0.0 and still be considered *cis*.
Example: '30.0'. **[struct_mon_details]**

**_struct_mon_details.RSCC** (*text*)

This data item describes the specifics of the calculations that generated the values given in **_struct_mon_prot.RSCC_all**, **_struct_mon_prot.RSCC_main** and **_struct_mon_prot.RSCC_side**. The coefficients used to calculate the $p(o)$ and $p(c)$ maps should be given as well as the criterion for the inclusion of map grid points in the calculation.

Examples:

```
; The map p(o) was calculated with coefficients
  2F(o) - F(c) and with phase alpha(c). F(o)
  are the observed structure-factor amplitudes,
  F(c) are the amplitudes calculated from the
  current model and alpha(c) are the phases
  calculated from the current model.
  The map p(c) was calculated in program O using
  a Gaussian distribution function around the
  atoms in the current model.
  Map grid points within 1.5 A of the
  designated atoms were included in the
  calculation.
;
; The map p(o) was calculated with coefficients
  F(o) and with phase alpha(c). F(o) are the
  observed structure-factor amplitudes, and
  alpha(c) are the phases calculated from the
  current model.
  The map p(c) was calculated with coefficients
  F(c) and with phases alpha(c). F(c) and
  alpha(c) are the structure-factor amplitudes
  and phases, respectively, calculated from the
  current model.
  Map grid points within a van der Waals radius
  of the designated atoms were included in the
  calculation.
;
```

**[struct_mon_details]**

**_struct_mon_details.RSR** (*text*)

This data item describes the specifics of the calculations that generated the values given in **_struct_mon_prot.RSR_all**, **_struct_mon_prot.RSR_main** and **_struct_mon_prot.RSR_side**. The coefficients used to calculate the $p(o)$ and $p(c)$ maps should be given as well as the criterion for the inclusion of map grid points in the calculation.

Examples:

```
; The map p(o) was calculated with coefficients
  2F(o) - F(c) and with phase alpha(c). F(o)
  are the observed structure-factor amplitudes,
  F(c) are the amplitudes calculated from the
  current model and alpha(c) are the phases
  calculated from the current model.
  The map p(c) was calculated in program O using
  a Gaussian distribution function around the
  atoms in the current model.
  Map grid points within 1.5 A of the
  designated atoms were included in the
  calculation.
;
; The map p(o) was calculated with coefficients
  F(o) and with phase alpha(c). F(o) are the
  observed structure-factor amplitudes, and
  alpha(c) are the phases calculated from the
  current model.
  The map p(c) was calculated with coefficients
  F(c) and with phases alpha(c). F(c) and
  alpha(c) are the structure-factor amplitudes
  and phases, respectively, calculated from the
  current model.
  Map grid points within a van der Waals radius
  of the designated atoms were included in the
  calculation.
;
```

**[struct_mon_details]**

## STRUCT_MON_NUCL

Data items in the STRUCT_MON_NUCL category record details about structural properties of a nucleic acid when analyzed at the monomer level. Analogous data items for proteins are given in the STRUCT_MON_PROT category. For items where the value of the property depends on the method employed to calculate it, details of the method of calculation are given using data items in the STRUCT_MON_DETAILS category.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct_mon_nucl.label_alt_id**
**_struct_mon_nucl.label_asym_id**
**_struct_mon_nucl.label_comp_id**
**_struct_mon_nucl.label_seq_id**

*Example 1 – based on NDB structure BDL028.*

```
loop_
_struct_mon_nucl.label_comp_id
_struct_mon_nucl.label_seq_id
_struct_mon_nucl.label_asym_id
_struct_mon_nucl.label_alt_id
_struct_mon_nucl.alpha
_struct_mon_nucl.beta
_struct_mon_nucl.gamma
_struct_mon_nucl.delta
_struct_mon_nucl.epsilon
_struct_mon_nucl.zeta
C  1 A .      .      .   29.9  131.9  222.1  174.2
G  2 A .  334.0  130.6   33.1  125.6  167.6  270.9
T  3 A .  258.2  178.7   101.0 114.6  216.6  259.3
#         ---- abbreviated list -----
```

**_struct_mon_nucl.alpha** (*float*)

The value in degrees of the backbone torsion angle $\alpha$ (O3′—P—O5′—C5′).

**[struct_mon_nucl]**

**_struct_mon_nucl.auth_asym_id**

A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_mon_nucl.auth_comp_id**

A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_mon_nucl.auth_seq_id**

A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_struct_mon_nucl.beta** (*float*)

The value in degrees of the backbone torsion angle $\beta$ (P—O5′—C5′—C4′).

**[struct_mon_nucl]**

**_struct_mon_nucl.chi1** (*float*)

The value in degrees of the sugar–base torsion angle $\chi_1$ (O4′—C1′—N1—C2).

**[struct_mon_nucl]**

**_struct_mon_nucl.chi2** (*float*)

The value in degrees of the sugar–base torsion angle $\chi_2$ (O4′—C1′—N9—C4).

**[struct_mon_nucl]**

**_struct_mon_nucl.delta** (*float*)
The value in degrees of the backbone torsion angle $\delta$ (C5′—C4′—C3′—O3′).

[struct_mon_nucl]

**_struct_mon_nucl.details** (*float*)
A description of special aspects of the residue, its conformation, behaviour in refinement, or any other aspect that requires annotation.

Example:
```
; Part of the phosphodiester backbone not in density.
;
```
[struct_mon_nucl]

**_struct_mon_nucl.epsilon** (*float*)
The value in degrees of the backbone torsion angle $\varepsilon$ (C4′—C3′—O3′—P).

[struct_mon_nucl]

**_struct_mon_nucl.gamma** (*float*)
The value in degrees of the backbone torsion angle $\gamma$ (O5′—C5′—C4′—C3′).

[struct_mon_nucl]

***_struct_mon_nucl.label_alt_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_struct_mon_nucl.label_asym_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_mon_nucl.label_comp_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_mon_nucl.label_seq_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_mon_nucl.mean_B_all** (*float*)
The mean value of the isotropic displacement parameter for all atoms in the monomer.

[struct_mon_nucl]

**_struct_mon_nucl.mean_B_base** (*float*)
The mean value of the isotropic displacement parameter for atoms in the base moiety of the nucleic acid monomer.

[struct_mon_nucl]

**_struct_mon_nucl.mean_B_phos** (*float*)
The mean value of the isotropic displacement parameter for atoms in the phosphate moiety of the nucleic acid monomer.

[struct_mon_nucl]

**_struct_mon_nucl.mean_B_sugar** (*float*)
The mean value of the isotropic displacement parameter for atoms in the sugar moiety of the nucleic acid monomer.

[struct_mon_nucl]

**_struct_mon_nucl.nu0** (*float*)
The value in degrees of the sugar torsion angle $\nu_0$ (C4′—O4′—C1′—C2′).

[struct_mon_nucl]

**_struct_mon_nucl.nu1** (*float*)
The value in degrees of the sugar torsion angle $\nu_1$ (O4′—C1′—C2′—C3′).

[struct_mon_nucl]

**_struct_mon_nucl.nu2** (*float*)
The value in degrees of the sugar torsion angle $\nu_2$ (C1′—C2′—C3′—C4′).

[struct_mon_nucl]

**_struct_mon_nucl.nu3** (*float*)
The value in degrees of the sugar torsion angle $\nu_3$ (C2′—C3′—C4′—O4′).

[struct_mon_nucl]

**_struct_mon_nucl.nu4** (*float*)
The value in degrees of the sugar torsion angle $\nu_4$ (C3′—C4′—O4′—C1′).

[struct_mon_nucl]

**_struct_mon_nucl.P** (*float*)
$P$ is the phase angle of pseudorotation for five-membered rings. For ribose and deoxyribose sugars in nucleic acids

$$P = \arctan\left(\frac{(\tau_4+\tau_1)-(\tau_3+\tau_0)}{2\tau_2(\sin 36+\sin 72)}\right).$$

If $\tau_2$ is $< 0$, then $P = P + 180^\circ$ (Altona & Sundaralingam, 1972).

Reference: Altona, C. & Sundaralingam, M. (1972). *J. Am. Chem. Soc.* **94**, 8205–8212.

[struct_mon_nucl]

**_struct_mon_nucl.RSCC_all** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the nucleic acid monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|}{(\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|^2)^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.

[struct_mon_nucl]

**_struct_mon_nucl.RSCC_base** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the base moiety of the nucleic acid monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|}{(\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|^2)^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSCC_phos** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the phosphate moiety of the nucleic acid monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|}{(\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|^2)^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSCC_sugar** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the sugar moiety of the nucleic acid monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|}{(\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}} \rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}} \rangle|^2)^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSR_all** (*float*)
The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the nucleic acid monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSR_base** (*float*)
The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the base moiety of the nucleic acid monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSR_phos** (*float*)
The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the phosphate moiety of the nucleic acid monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_nucl]**

**_struct_mon_nucl.RSR_sugar** (*float*)
The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the sugar moiety of the nucleic acid monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_nucl]**

**_struct_mon_nucl.tau0** (*float*)
The value in degrees of the sugar torsion angle $\tau_0$ (C4′—O4′—C1′—C2′).

[struct_mon_nucl]

**_struct_mon_nucl.tau1** (*float*)
The value in degrees of the sugar torsion angle $\tau_1$ (O4′—C1′—C2′—C3′).

[struct_mon_nucl]

**_struct_mon_nucl.tau2** (*float*)
The value in degrees of the sugar torsion angle $\tau_2$ (C1′—C2′—C3′—C4′).

[struct_mon_nucl]

**_struct_mon_nucl.tau3** (*float*)
The value in degrees of the sugar torsion angle $\tau_3$ (C2′—C3′—C4′—O4′).

[struct_mon_nucl]

**_struct_mon_nucl.tau4** (*float*)
The value in degrees of the sugar torsion angle $\tau_4$ (C3′—C4′—O4′—C1′).

[struct_mon_nucl]

**_struct_mon_nucl.taum** (*float*)
The maximum amplitude of puckering. This is derived from the pseudorotation value $P$ and the torsion angles in the ribose ring.

$$\tau_2 = \tau_m \cos P,$$
$$\tau_3 = \tau_m \cos(P + 144),$$
$$\tau_4 = \tau_m \cos(P + 288),$$
$$\tau_0 = \tau_m \cos(P + 72),$$
$$\tau_1 = \tau_m \cos(P + 216).$$

[struct_mon_nucl]

**_struct_mon_nucl.zeta** (*float*)
The value in degrees of the backbone torsion angle $\zeta$ (C3′—O3′—P—O5′).

[struct_mon_nucl]

## STRUCT_MON_PROT

Data items in the STRUCT_MON_PROT category record details about structural properties of a protein when analyzed at the monomer level. Analogous data items for nucleic acids are given in the STRUCT_MON_NUCL category. For items where the value of the property depends on the method employed to calculate it, details of the method of calculation are given using data items in the STRUCT_MON_DETAILS category.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_mon_prot.label_alt_id**
**_struct_mon_prot.label_asym_id**
**_struct_mon_prot.label_comp_id**
**_struct_mon_prot.label_seq_id**

*Example 1 – based on laboratory records for protein NS1. This example provides details for residue ARG 35.*

```
_struct_mon_prot.label_comp_id   ARG
_struct_mon_prot.label_seq_id     35
_struct_mon_prot.label_asym_id     A
_struct_mon_prot.label_alt_id      .
_struct_mon_prot.chi1           -67.9
_struct_mon_prot.chi2          -174.7
_struct_mon_prot.chi3           -67.7
_struct_mon_prot.chi4           -86.3
_struct_mon_prot.chi5             4.2
_struct_mon_prot.RSCC_all         0.90
_struct_mon_prot.RSR_all          0.18
_struct_mon_prot.mean_B_all       30.0
_struct_mon_prot.mean_B_main      25.0
_struct_mon_prot.mean_B_side      35.1
_struct_mon_prot.omega           180.1
_struct_mon_prot.phi             -60.3
_struct_mon_prot.psi             -46.0
```

**_struct_mon_prot.auth_asym_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_mon_prot.auth_comp_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_mon_prot.auth_seq_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_struct_mon_prot.chi1** (*float*)
The value in degrees of the side-chain torsion angle $\chi_1$, for those residues containing such an angle.

[struct_mon_prot]

**_struct_mon_prot.chi2** (*float*)
The value in degrees of the side-chain torsion angle $\chi_2$, for those residues containing such an angle.

[struct_mon_prot]

**_struct_mon_prot.chi3** (*float*)
The value in degrees of the side-chain torsion angle $\chi_3$, for those residues containing such an angle.

[struct_mon_prot]

**_struct_mon_prot.chi4** (*float*)
The value in degrees of the side-chain torsion angle $\chi_4$, for those residues containing such an angle.

[struct_mon_prot]

**_struct_mon_prot.chi5** (*float*)
The value in degrees of the side-chain torsion angle $\chi_5$, for those residues containing such an angle.

[struct_mon_prot]

**_struct_mon_prot.details** (*float*)
A description of special aspects of the residue, its conformation, behaviour in refinement, or any other aspect that requires annotation.

Examples: 'very poor density',
```
; The side chain of this density may occupy alternative
conformations, but alternative conformations were not fit
in this model.
;
; This residue has a close contact with the bound inhibitor,
which may account for the nonstandard conformation of the
side chain.
;
```
**[struct_mon_prot]**

* **_struct_mon_prot.label_alt_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

* **_struct_mon_prot.label_asym_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

* **_struct_mon_prot.label_comp_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

* **_struct_mon_prot.label_seq_id**
A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_mon_prot.mean_B_all** (*float*)
The mean value of the isotropic displacement parameter for all atoms in the monomer.
**[struct_mon_prot]**

**_struct_mon_prot.mean_B_main** (*float*)
The mean value of the isotropic displacement parameter for atoms in the main chain of the monomer.
**[struct_mon_prot]**

**_struct_mon_prot.mean_B_side** (*float*)
The mean value of the isotropic displacement parameter for atoms in the side chain of the monomer.
**[struct_mon_prot]**

**_struct_mon_prot.omega** (*float*)
The value in degrees of the main-chain torsion angle $\omega$.
**[struct_mon_prot]**

**_struct_mon_prot.phi** (*float*)
The value in degrees of the main-chain torsion angle $\varphi$.
**[struct_mon_prot]**

**_struct_mon_prot.psi** (*float*)
The value in degrees of the main-chain torsion angle $\psi$.
**[struct_mon_prot]**

**_struct_mon_prot.RSCC_all** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|}{(\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|^2)^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.
**[struct_mon_prot]**

**_struct_mon_prot.RSCC_main** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the main chain of the monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|}{[\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|^2]^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.
**[struct_mon_prot]**

**_struct_mon_prot.RSCC_side** (*float*)
The real-space (linear) correlation coefficient RSCC, as described by Jones *et al.* (1991), evaluated over all atoms in the side chain of the monomer.

$$\mathrm{RSCC} = \frac{\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle| \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|}{[\sum |p_{\mathrm{obs}} - \langle p_{\mathrm{obs}}\rangle|^2 \sum |p_{\mathrm{calc}} - \langle p_{\mathrm{calc}}\rangle|^2]^{1/2}},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSCC**. $\langle\rangle$ indicates an average and the sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSCC**.

Reference: Jones, T. A., Zou, J.-Y., Cowan, S. W. & Kjeldgaard, M. (1991). *Acta Cryst.* A**47**, 110–119.
**[struct_mon_prot]**

**_struct_mon_prot.RSR_all** (*float*)
The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken

over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_prot]**

**_struct_mon_prot.RSR_main** (*float*)

The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the main chain of the monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_prot]**

**_struct_mon_prot.RSR_side** (*float*)

The real-space residual RSR, as described by Brändén & Jones (1990), evaluated over all atoms in the side chain of the monomer.

$$\mathrm{RSR} = \frac{\sum |p_{\mathrm{obs}} - p_{\mathrm{calc}}|}{\sum |p_{\mathrm{obs}} + p_{\mathrm{calc}}|},$$

where $p_{\mathrm{obs}}$ = the density in an 'experimental' map, $p_{\mathrm{calc}}$ = the density in a 'calculated' map and the sum is taken over the specified grid points. Details of how these maps were calculated should be given in **_struct_mon_details.RSR**. The sums are taken over all map grid points near the relevant atoms. The radius for including grid points in the calculation should also be given in **_struct_mon_details.RSR**.

Reference: Brändén, C.-I. & Jones, T. A. (1990). *Nature (London)*, **343**, 687–689.

**[struct_mon_prot]**

## STRUCT_MON_PROT_CIS

Data items in the STRUCT_MON_PROT_CIS category identify monomers that have been found to have the peptide bond in the *cis* conformation. The criterion used to select residues to be designated as containing *cis* peptide bonds is given in **_struct_mon_details.prot_cis**.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_mon_prot_cis.label_alt_id**
**_struct_mon_prot_cis.label_asym_id**
**_struct_mon_prot_cis.label_comp_id**
**_struct_mon_prot_cis.label_seq_id**

*Example 1 – based on PDB structure 1ACY of Ghiara, Stura, Stanfield, Profy & Wilson [Science (1994), **264**, 82–85].*

```
loop_
_struct_mon_prot_cis.label_comp_id
_struct_mon_prot_cis.label_seq_id
_struct_mon_prot_cis.label_asym_id
_struct_mon_prot_cis.label_alt_id
 PRO   8  L .
 PRO  77  L .
 PRO  95  L .
 PRO 141  L .
 #  -----   abbreviated  -----
```

**_struct_mon_prot_cis.auth_asym_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_mon_prot_cis.auth_comp_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_mon_prot_cis.auth_seq_id**

A component of the identifier for the monomer.This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

***_struct_mon_prot_cis.label_alt_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_struct_mon_prot_cis.label_asym_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_mon_prot_cis.label_comp_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_mon_prot_cis.label_seq_id**

A component of the identifier for the monomer. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

## STRUCT_NCS_DOM

Data items in the STRUCT_NCS_DOM category record information about the domains in an ensemble of domains related by one or more noncrystallographic symmetry operators. A domain need not correspond to a complete polypeptide chain; it can be composed of one or more segments in a single chain, or by segments from more than one chain.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_ncs_dom.id**

*Example 1 – based on laboratory records for the collagen-like peptide, HYP-.*

```
loop_
_struct_ncs_dom.id
_struct_ncs_dom.details
 d1  'Chains A, B, and C'
 d2  'Chains D, E, and F'
```

**_struct_ncs_dom.details** (*text*)

A description of special aspects of the structural elements that comprise a domain in an ensemble of domains related by noncrystallographic symmetry.

Example:

```
; The loop between residues 18 and 23 in this domain interacts
with a symmetry-related molecule, and thus deviates
significantly from the noncrystallographic threefold.
;
```

**[struct_ncs_dom]**

*`_struct_ncs_dom.id` (*code*)
The value of `_struct_ncs_dom.id` must uniquely identify a record in the STRUCT_NCS_DOM list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

*`_struct_ncs_dom_lim.dom_id`*,
*`_struct_ncs_ens_gen.dom_id_1`*,
*`_struct_ncs_ens_gen.dom_id_2`*. `[struct_ncs_dom]`

## STRUCT_NCS_DOM_LIM

Data items in the STRUCT_NCS_DOM_LIM category identify the start and end points of polypeptide chain segments that form all or part of a domain in an ensemble of domains related by non-crystallographic symmetry.

Category group(s): `inclusive_group`
`struct_group`
Category key(s): `_struct_ncs_dom_lim.dom_id`
`_struct_ncs_dom_lim.beg_label_alt_id`
`_struct_ncs_dom_lim.beg_label_asym_id`
`_struct_ncs_dom_lim.beg_label_comp_id`
`_struct_ncs_dom_lim.beg_label_seq_id`
`_struct_ncs_dom_lim.end_label_alt_id`
`_struct_ncs_dom_lim.end_label_asym_id`
`_struct_ncs_dom_lim.end_label_comp_id`
`_struct_ncs_dom_lim.end_label_seq_id`

*Example 1 – based on laboratory records for the collagen-like peptide, HYP-.*

```
loop_
_struct_ncs_dom_lim.dom_id
_struct_ncs_dom_lim.beg_label_alt_id
_struct_ncs_dom_lim.beg_label_asym_id
_struct_ncs_dom_lim.beg_label_comp_id
_struct_ncs_dom_lim.beg_label_seq_id
_struct_ncs_dom_lim.end_label_alt_id
_struct_ncs_dom_lim.end_label_asym_id
_struct_ncs_dom_lim.end_label_comp_id
_struct_ncs_dom_lim.end_label_seq_id
 d1   .  A PRO  1   . A GLY  29
 d1   .  B PRO  31  . B GLY  59
 d1   .  C PRO  61  . B GLY  89
 d2   .  D PRO  91  . D GLY 119
 d2   .  E PRO 121  . E GLY 149
 d2   .  F PRO 151  . F GLY 179
```

**`_struct_ncs_dom_lim.beg_auth_asym_id`**
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.auth_asym_id` in the ATOM_SITE category.

**`_struct_ncs_dom_lim.beg_auth_comp_id`**
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.auth_comp_id` in the ATOM_SITE category.

**`_struct_ncs_dom_lim.beg_auth_seq_id`**
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.auth_seq_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.beg_label_alt_id`
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_sites_alt.id` in the ATOM_SITES_ALT category.

*`_struct_ncs_dom_lim.beg_label_asym_id`
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.label_asym_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.beg_label_comp_id`
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.label_comp_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.beg_label_seq_id`
A component of the identifier for the monomer at which this segment of the domain begins. This data item is a pointer to `_atom_site.label_seq_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.dom_id`
This data item is a pointer to `_struct_ncs_dom.id` in the STRUCT_NCS_DOM category.

**`_struct_ncs_dom_lim.end_auth_asym_id`**
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.auth_asym_id` in the ATOM_SITE category.

**`_struct_ncs_dom_lim.end_auth_comp_id`**
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.auth_comp_id` in the ATOM_SITE category.

**`_struct_ncs_dom_lim.end_auth_seq_id`**
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.auth_seq_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.end_label_alt_id`
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_sites_alt.id` in the ATOM_SITES_ALT category.

*`_struct_ncs_dom_lim.end_label_asym_id`
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.label_asym_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.end_label_comp_id`
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.label_comp_id` in the ATOM_SITE category.

*`_struct_ncs_dom_lim.end_label_seq_id`
A component of the identifier for the monomer at which this segment of the domain ends. This data item is a pointer to `_atom_site.label_seq_id` in the ATOM_SITE category.

## STRUCT_NCS_ENS

Data items in the STRUCT_NCS_ENS category record information about ensembles of domains related by noncrystallographic symmetry. The point group of the ensemble when taken as a whole may be specified, as well as any special aspects of the ensemble that require description.

Category group(s): `inclusive_group`
`struct_group`
Category key(s): `_struct_ncs_ens.id`

*Example 1 – based on laboratory records for the collagen-like peptide, HYP-.*

```
_struct_ncs_ens.id          en1
_struct_ncs_ens.details
; The ensemble represents the pseudo-twofold symmetry
  between domains d1 and d2.
;
```

**_struct_ncs_ens.details** (*text*)

A description of special aspects of the ensemble.

Example:

```
; The ensemble has a slight translation between domains 1
and 4, but overall it can accurately be described as point
group 222
;
```

**[struct_ncs_ens]**

***_struct_ncs_ens.id** (*code*)

The value of **_struct_ncs_ens.id** must uniquely identify a record in the STRUCT_NCS_ENS list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_struct_ncs_ens_gen.ens_id***.

**[struct_ncs_ens]**

**_struct_ncs_ens.point_group** (*line*)

The point group of the ensemble of structural elements related by one or more noncrystallographic symmetry operations. The relationships need not be precise; this data item is intended to give a rough description of the noncrystallographic symmetry relationships.

Examples: '3', '422', 'non-proper'.

**[struct_ncs_ens]**

## STRUCT_NCS_ENS_GEN

Data items in the STRUCT_NCS_ENS_GEN category list domains related by a noncrystallographic symmetry operation and identify the operator.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct_ncs_ens_gen.ens_id**
**_struct_ncs_ens_gen.dom_id_1**
**_struct_ncs_ens_gen.dom_id_2**
**_struct_ncs_ens_gen.oper_id**

*Example 1 – based on laboratory records for the collagen-like peptide, HYP-.*

```
_struct_ncs_ens_gen.dom_id_1  d1
_struct_ncs_ens_gen.dom_id_2  d2
_struct_ncs_ens_gen.ens_id    en1
_struct_ncs_ens_gen.oper_id   ncsop1
```

***_struct_ncs_ens_gen.dom_id_1**

The identifier for the domain that will remain unchanged by the transformation operator. This data item is a pointer to **_struct_ncs_dom.id** in the STRUCT_NCS_DOM category.

***_struct_ncs_ens_gen.dom_id_2**

The identifier for the domain that will be transformed by application of the transformation operator. This data item is a pointer to **_struct_ncs_dom.id** in the STRUCT_NCS_DOM category.

***_struct_ncs_ens_gen.ens_id**

This data item is a pointer to **_struct_ncs_ens.id** in the STRUCT_NCS_ENS category.

***_struct_ncs_ens_gen.oper_id**

This data item is a pointer to **_struct_ncs_oper.id** in the STRUCT_NCS_OPER category.

## STRUCT_NCS_OPER

Data items in the STRUCT_NCS_OPER category describe the noncrystallographic symmetry operations. Each operator is specified as a matrix and a subsequent translation vector. Operators need not represent proper rotations.

Category group(s): **inclusive_group**
**struct_group**

Category key(s): **_struct_ncs_oper.id**

*Example 1 – based on laboratory records for the protein NS1.*

```
_struct_ncs_oper.id             ncsop1
_struct_ncs_oper.code           given
_struct_ncs_oper.matrix[1][1]   0.247
_struct_ncs_oper.matrix[1][2]   0.935
_struct_ncs_oper.matrix[1][3]   0.256
_struct_ncs_oper.matrix[2][1]   0.929
_struct_ncs_oper.matrix[2][2]   0.153
_struct_ncs_oper.matrix[2][3]   0.337
_struct_ncs_oper.matrix[3][1]   0.276
_struct_ncs_oper.matrix[3][2]   0.321
_struct_ncs_oper.matrix[3][3]  -0.906
_struct_ncs_oper.vector[1]     -8.253
_struct_ncs_oper.vector[2]    -11.743
_struct_ncs_oper.vector[3]     -1.782
_struct_ncs_oper.details
; Matrix and translation vector for pseudo-twofold operation.
;
```

**_struct_ncs_oper.code** (*code*)

A code to indicate whether this operator describes a relationship between coordinates all of which are given in the data block (in which case the value of code is 'given'), or whether the operator is used to generate new coordinates from those that are given in the data block (in which case the value of code is 'generate').

The data value must be one of the following:

| | |
|---|---|
| given | operator relates coordinates given in the data block |
| generate | operator generates new coordinates from those given in the data block |

**[struct_ncs_oper]**

**_struct_ncs_oper.details** (*text*)

A description of special aspects of the noncrystallographic symmetry operator.

Example:

```
; The operation is given as a precise threefold rotation,
despite the fact the best rms fit between domain 1 and domain
2 yields a rotation of 119.7 degrees and a translation of
0.13 angstroms.
;
```

**[struct_ncs_oper]**

***_struct_ncs_oper.id** (*code*)

The value of **_struct_ncs_oper.id** must uniquely identify a record in the STRUCT_NCS_OPER list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*

***_struct_ncs_ens_gen.oper_id***.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[1][1]** (*float*)

The [1][1] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[1][2]** (*float*)

The [1][2] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[1][3]** (*float*)

The [1][3] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[2][1]** (*float*)
The [2][1] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[2][2]** (*float*)
The [2][2] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[2][3]** (*float*)
The [2][3] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[3][1]** (*float*)
The [3][1] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[3][2]** (*float*)
The [3][2] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.matrix[3][3]** (*float*)
The [3][3] element of the 3 × 3 matrix component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.vector[1]** (*float*)
The [1] element of the three-element vector component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.vector[2]** (*float*)
The [2] element of the three-element vector component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

**_struct_ncs_oper.vector[3]** (*float*)
The [3] element of the three-element vector component of a noncrystallographic symmetry operation.

**[struct_ncs_oper]**

## STRUCT_REF

Data items in the STRUCT_REF category allow the author of a data block to relate the entities or biological units described in the data block to information archived in external databases. For references to the sequence of a polymer, the value of the data item **_struct_ref.seq_align** is used to indicate whether the correspondence between the sequence of the entity or biological unit in the data block and the sequence in the referenced database entry is 'complete' or 'partial'. If this value is 'partial', the region (or regions) of the alignment may be delimited using data items in the STRUCT_REF_SEQ category. Similarly, the value of **_struct_ref.seq_dif** is used to indicate whether the two sequences contain point differences. If the value is 'yes', the differences may be identified and annotated using data items in the STRUCT_REF_SEQ_DIF category.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_ref.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_ref.id
_struct_ref.entity_id
_struct_ref.biol_id
_struct_ref.db_name
_struct_ref.db_code
_struct_ref.seq_align
_struct_ref.seq_dif
_struct_ref.details
 seq_pdb     .  1  PDB      5HVP      .         .
; The structure of the closely related compound,
  isobutyryl-pepstatin (pepstatin A) in complex with
  rhizopuspepsin
;
 seq_genbank 1  .  GenBank  AAG30358  complete  yes  .
```

**_struct_ref.biol_id**
This data item is a pointer to **_struct_biol.id** in the STRUCT_BIOL category.

* **_struct_ref.db_code** (*line*)
The code for this entity or biological unit or for a closely related entity or biological unit in the named database.
Examples: '1ABC', 'ABCDEF'. **[struct_ref]**

* **_struct_ref.db_name** (*line*)
The name of the database containing reference information about this entity or biological unit.
Examples: 'PDB', 'CSD', 'Genbank'. **[struct_ref]**

**_struct_ref.details** (*text*)
A description of special aspects of the relationship between the entity or biological unit described in the data block and that in the referenced database entry.

**[struct_ref]**

* **_struct_ref.entity_id**
This data item is a pointer to **_entity.id** in the ENTITY category.

* **_struct_ref.id** (*code*)
The value of **_struct_ref.id** must uniquely identify a record in the STRUCT_REF list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_struct_ref_seq.ref_id***. **[struct_ref]**

**_struct_ref.seq_align** (*ucode*)
A flag to indicate the scope of the alignment between the sequence of the entity or biological unit described in the data block and that in the referenced database entry. 'complete' indicates that alignment spans the entire length of both sequences (although point differences may occur and can be annotated using the data items in the STRUCT_REF_SEQ_DIF category). 'partial' indicates a partial alignment. The region (or regions) of the alignment may be delimited using data items in the STRUCT_REF_SEQ category. This data item may also take the value '.', indicating that the reference is not to a sequence.
The data value must be one of the following:

| | |
|---|---|
| complete | alignment is complete |
| partial | alignment is partial |
| . | reference is not to a sequence |

**[struct_ref]**

**_struct_ref.seq_dif** (*ucode*)
A flag to indicate the presence ('yes') or absence ('no') of point differences between the sequence of the entity or biological unit described in the data block and that in the referenced database entry. This data item may also take the value '.', indicating that the reference is not to a sequence.

The data value must be one of the following:

| | |
|---|---|
| no | there are no point differences |
| n | abbreviation for 'no' |
| yes | there are point difference |
| y | abbreviation for 'yes' |
| . | reference is not to a sequence |

**[struct_ref]**

## STRUCT_REF_SEQ

Data items in the STRUCT_REF_SEQ category provide a mechanism for indicating and annotating a region (or regions) of alignment between the sequence of an entity or biological unit described in the data block and the sequence in the referenced database entry.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_ref_seq.align_id**

*Example 1 – based on the sequence alignment of CHER from M. xantus (36 to 288) and CHER from S. typhimurium (18 to 276).*

```
_struct_ref_seq.align_id          alg1
_struct_ref_seq.ref_id            seqdb1
_struct_ref_seq.seq_align_beg     36
_struct_ref_seq.seq_align_end     288
_struct_ref_seq.db_align_beg      18
_struct_ref_seq.db_align_end      276
_struct_ref_seq.details
; The alignment contains 3 gaps larger than 2 residues
;
```

***_struct_ref_seq.align_id** (*code*)
The value of **_struct_ref_seq.align_id** must uniquely identify a record in the STRUCT_REF_SEQ list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*
***_struct_ref_seq_dif.align_id***. **[struct_ref_seq]**

***_struct_ref_seq.db_align_beg** (*int*)
The sequence position in the referenced database entry at which the alignment begins.

***_struct_ref_seq.db_align_end** (*int*)
The sequence position in the referenced database entry at which the alignment ends.

**_struct_ref_seq.details** (*text*)
A description of special aspects of the sequence alignment.
**[struct_ref_seq]**

***_struct_ref_seq.ref_id**
This data item is a pointer to **_struct_ref.id** in the STRUCT_REF category.

***_struct_ref_seq.seq_align_beg**
The sequence position in the entity or biological unit described in the data block at which the alignment begins. This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

***_struct_ref_seq.seq_align_end**
The sequence position in the entity or biological unit described in the data block at which the alignment ends. This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

## STRUCT_REF_SEQ_DIF

Data items in the STRUCT_REF_SEQ_DIF category provide a mechanism for indicating and annotating point differences between the sequence of the entity or biological unit described in the data block and the sequence of the referenced database entry.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_ref_seq_dif.align_id**
**_struct_ref_seq_dif.seq_num**

*Example 1 – based on laboratory records for CAP-DNA complex.*

```
_struct_ref_seq_dif.align_id   algn2
_struct_ref_seq_dif.seq_num    181
_struct_ref_seq_dif.db_mon_id  GLU
_struct_ref_seq_dif.mon_id     PHE
_struct_ref_seq_dif.details
; A point mutation was introduced in the CAP at position 181
  substituting PHE for GLU.
;
```

***_struct_ref_seq_dif.align_id**
This data item is a pointer to **_struct_ref_seq.align_id** in the STRUCT_REF_SEQ category.

***_struct_ref_seq_dif.db_mon_id**
The monomer type found at this position in the referenced database entry. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

**_struct_ref_seq_dif.details** (*text*)
A description of special aspects of the point differences between the sequence of the entity or biological unit described in the data block and that in the referenced database entry.
**[struct_ref_seq_dif]**

***_struct_ref_seq_dif.mon_id**
The monomer type found at this position in the sequence of the entity or biological unit described in this data block. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

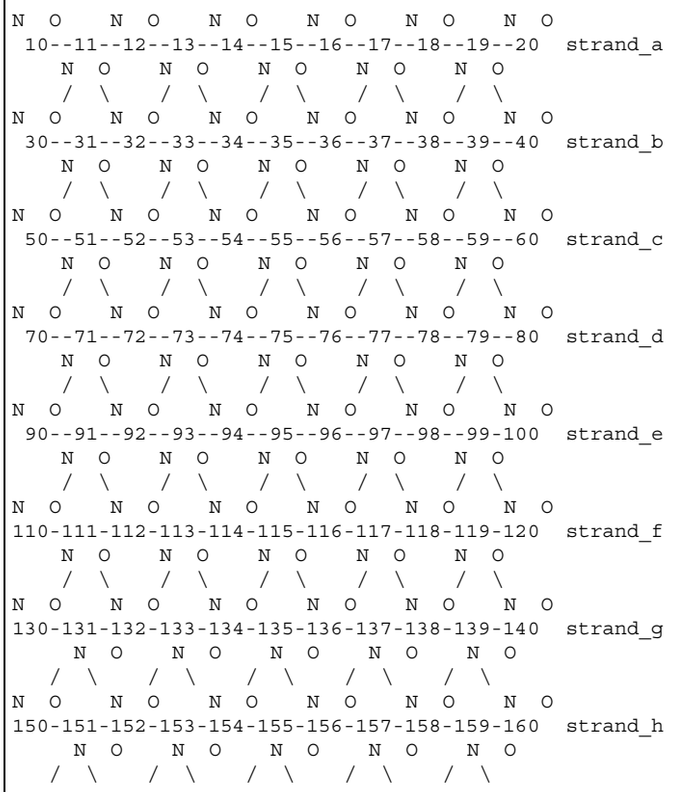
***_struct_ref_seq_dif.seq_num**
This data item is a pointer to **_entity_poly_seq.num** in the ENTITY_POLY_SEQ category.

## STRUCT_SHEET

Data items in the STRUCT_SHEET category record details about the $\beta$-sheets.

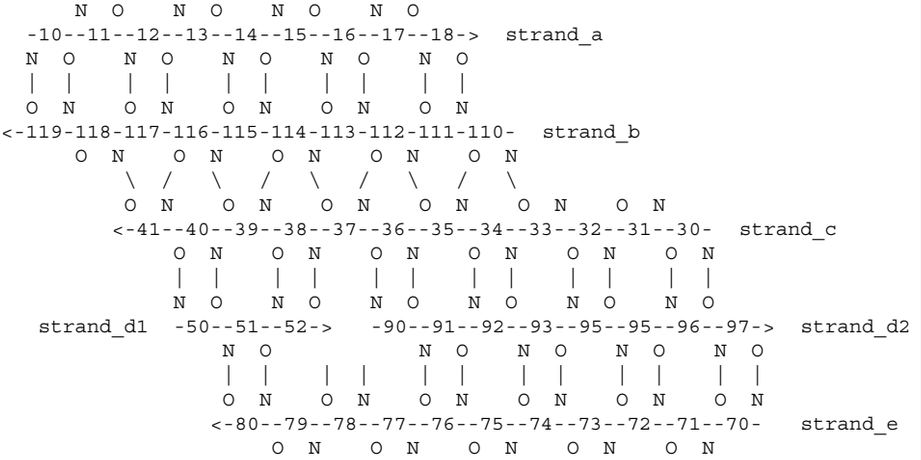
Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_sheet.id**

*Example 1 - simple beta-barrel.*




```
_struct_sheet.id               sheet_1
_struct_sheet.type            'beta-barrel'
_struct_sheet.number_strands   8
_struct_sheet.details          .
```

*Example 2 - five stranded mixed-sense sheet with one two-piece strand.*




```
_struct_sheet.id               sheet_2
_struct_sheet.type            'five stranded, mixed-sense'
_struct_sheet.number_strands   5
_struct_sheet.details         'strand_d is in two pieces'
```

**_struct_sheet.details** (*text*)
A description of special aspects of the $\beta$-sheet.
**[struct_sheet]**

***_struct_sheet.id** (*code*)
The value of **_struct_sheet.id** must uniquely identify a record in the STRUCT_SHEET list. Note that this item need not be a number; it can be any unique identifier.
*The following item(s) have an equivalent role in their respective categories:*
***_struct_sheet_hbond.sheet_id***,
***_struct_sheet_order.sheet_id***,
***_struct_sheet_range.sheet_id***,
***_struct_sheet_topology.sheet_id***. **[struct_sheet]**

**_struct_sheet.number_strands** (*int*)
The number of strands in the sheet. If a given range of residues bulges out from the strands, it is still counted as one strand. If a strand is composed of two different regions of polypeptide, it is still counted as one strand, as long as the proper hydrogen-bonding connections are made to adjacent strands.
**[struct_sheet]**

**_struct_sheet.type** (*text*)
A simple descriptor for the type of the sheet.
Examples: 'jelly-roll', 'Rossmann fold', 'beta barrel'. **[struct_sheet]**

## STRUCT_SHEET_HBOND

Data items in the STRUCT_SHEET_HBOND category record details about the hydrogen bonding between residue ranges in a $\beta$-sheet. It is necessary to treat hydrogen bonding independently of the designation of ranges, because the hydrogen bonding may begin in different places for the interactions of a given strand with the one preceding it and the one following it in the sheet.
Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_sheet_hbond.sheet_id**
**_struct_sheet_hbond.range_id_1**
**_struct_sheet_hbond.range_id_2**

*Example 1 – simple beta-barrel.*

```
loop_
_struct_sheet_hbond.sheet_id
_struct_sheet_hbond.range_id_1
_struct_sheet_hbond.range_id_2
_struct_sheet_hbond.range_1_beg_label_seq_id
_struct_sheet_hbond.range_1_beg_label_atom_id
_struct_sheet_hbond.range_2_beg_label_seq_id
_struct_sheet_hbond.range_2_beg_label_atom_id
_struct_sheet_hbond.range_1_end_label_seq_id
_struct_sheet_hbond.range_1_end_label_atom_id
_struct_sheet_hbond.range_2_end_label_seq_id
_struct_sheet_hbond.range_2_end_label_atom_id
 sheet_1  strand_a  strand_b   11  N   30  O   19  O   40  N
 sheet_1  strand_b  strand_c   31  N   50  O   39  O   60  N
 sheet_1  strand_c  strand_d   51  N   70  O   59  O   80  N
 sheet_1  strand_d  strand_e   71  N   90  O   89  O  100  N
 sheet_1  strand_e  strand_f   91  N  110  O   99  O  120  N
 sheet_1  strand_f  strand_g  111  N  130  O  119  O  140  N
 sheet_1  strand_g  strand_h  131  N  150  O  139  O  160  N
 sheet_1  strand_h  strand_a  151  N   10  O  159  O  180  N
```

*Example 2 – five stranded mixed-sense sheet with one two-piece strand.*

```
loop_
_struct_sheet_hbond.sheet_id
_struct_sheet_hbond.range_id_1
_struct_sheet_hbond.range_id_2
_struct_sheet_hbond.range_1_beg_label_seq_id
_struct_sheet_hbond.range_1_beg_label_atom_id
_struct_sheet_hbond.range_2_beg_label_seq_id
_struct_sheet_hbond.range_2_beg_label_atom_id
_struct_sheet_hbond.range_1_end_label_seq_id
_struct_sheet_hbond.range_1_end_label_atom_id
_struct_sheet_hbond.range_2_end_label_seq_id
_struct_sheet_hbond.range_2_end_label_atom_id
 sheet_2  strand_a   strand_b    20  N  119  O  18  O  111  N
 sheet_2  strand_b   strand_c   110  N   33  O 118  N   41  O
 sheet_2  strand_c   strand_d1   38  N   52  O  40  O   50  N
 sheet_2  strand_c   strand_d2   30  N   96  O  36  O   90  N
 sheet_2  strand_d1  strand_e    51  N   80  O  51  O   80  N
 sheet_2  strand_d2  strand_e    91  N   76  O  97  O   70  N
```

**_struct_sheet_hbond.range_1_beg_auth_atom_id**
A component of the identifier for the residue for the first partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_1_beg_auth_seq_id**
A component of the identifier for the residue for the first partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

***_struct_sheet_hbond.range_1_beg_label_atom_id**
A component of the identifier for the residue for the first partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

***_struct_sheet_hbond.range_1_beg_label_seq_id**
A component of the identifier for the residue for the first partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_1_end_auth_atom_id**
A component of the identifier for the residue for the first partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_1_end_auth_seq_id**
A component of the identifier for the residue for the first partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

***_struct_sheet_hbond.range_1_end_label_atom_id**
A component of the identifier for the residue for the first partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

***_struct_sheet_hbond.range_1_end_label_seq_id**
A component of the identifier for the residue for the first partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_2_beg_auth_atom_id**
A component of the identifier for the residue for the second partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_2_beg_auth_seq_id**
A component of the identifier for the residue for the second partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

*__struct_sheet_hbond.range_2_beg_label_atom_id**
A component of the identifier for the residue for the second partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

*__struct_sheet_hbond.range_2_beg_label_seq_id**
A component of the identifier for the residue for the second partner of the first hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_2_end_auth_atom_id**
A component of the identifier for the residue for the second partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_sheet_hbond.range_2_end_auth_seq_id**
A component of the identifier for the residue for the second partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

*__struct_sheet_hbond.range_2_end_label_atom_id**
A component of the identifier for the residue for the second partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_atom_id** in the ATOM_SITE category.

*__struct_sheet_hbond.range_2_end_label_seq_id**
A component of the identifier for the residue for the second partner of the last hydrogen bond between two residue ranges in a sheet. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

*__struct_sheet_hbond.range_id_1**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

*__struct_sheet_hbond.range_id_2**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

*__struct_sheet_hbond.sheet_id**
This data item is a pointer to **_struct_sheet.id** in the STRUCT_SHEET category.

## STRUCT_SHEET_ORDER

Data items in the STRUCT_SHEET_ORDER category record details about the order of the residue ranges that form a $\beta$-sheet. All order links are pairwise and the specified pairs are assumed to be adjacent to one another in the sheet. These data items are an alternative to the STRUCT_SHEET_TOPOLOGY data items and they allow all manner of sheets to be described.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_sheet_order.sheet_id**
**_struct_sheet_order.range_id_1**
**_struct_sheet_order.range_id_2**

*Example 1 – simple beta-barrel.*

```
loop_
_struct_sheet_order.sheet_id
_struct_sheet_order.range_id_1
_struct_sheet_order.range_id_2
_struct_sheet_order.offset
_struct_sheet_order.sense
 sheet_1  strand_a  strand_b  +1  parallel
 sheet_1  strand_b  strand_c  +1  parallel
 sheet_1  strand_c  strand_d  +1  parallel
 sheet_1  strand_d  strand_e  +1  parallel
 sheet_1  strand_e  strand_f  +1  parallel
 sheet_1  strand_f  strand_g  +1  parallel
 sheet_1  strand_g  strand_h  +1  parallel
 sheet_1  strand_h  strand_a  +1  parallel
```

*Example 2 – five stranded mixed-sense sheet with one two-piece strand.*

```
loop_
_struct_sheet_order.sheet_id
_struct_sheet_order.range_id_1
_struct_sheet_order.range_id_2
_struct_sheet_order.offset
_struct_sheet_order.sense
 sheet_2  strand_a   strand_b    +1 anti-parallel
 sheet_2  strand_b   strand_c    +1 parallel
 sheet_2  strand_c   strand_d1   +1 anti-parallel
 sheet_2  strand_c   strand_d2   +1 anti-parallel
 sheet_2  strand_d1  strand_e    +1 anti-parallel
 sheet_2  strand_d2  strand_e    +1 anti-parallel
```

**_struct_sheet_order.offset** (*int*)
Designates the relative position in the sheet, plus or minus, of the second residue range to the first.
**[struct_sheet_order]**

*__struct_sheet_order.range_id_1**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

*__struct_sheet_order.range_id_2**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

**_struct_sheet_order.sense** (*ucode*)
A flag to indicate whether the two designated residue ranges are parallel or antiparallel to one another.
The data value must be one of the following:
parallel
anti-parallel
**[struct_sheet_order]**

*__struct_sheet_order.sheet_id**
This data item is a pointer to **_struct_sheet.id** in the STRUCT_SHEET category.

## STRUCT_SHEET_RANGE

Data items in the STRUCT_SHEET_RANGE category record details about the residue ranges that form a $\beta$-sheet. Residues are included in a range if they made $\beta$-sheet-type hydrogen-bonding interactions with at least one adjacent strand and if there are at least two residues in the range.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_sheet_range.sheet_id**
**_struct_sheet_range.id**

*Example 1 – simple beta-barrel.*

```
loop_
_struct_sheet_range.sheet_id
_struct_sheet_range.id
_struct_sheet_range.beg_label_comp_id
_struct_sheet_range.beg_label_asym_id
_struct_sheet_range.beg_label_seq_id
_struct_sheet_range.end_label_comp_id
_struct_sheet_range.end_label_asym_id
_struct_sheet_range.end_label_seq_id
_struct_sheet_range.symmetry
 sheet_1  strand_a  ala  A   20  ala  A   30  1_555
 sheet_1  strand_b  ala  A   40  ala  A   50  1_555
 sheet_1  strand_c  ala  A   60  ala  A   70  1_555
 sheet_1  strand_d  ala  A   80  ala  A   90  1_555
 sheet_1  strand_e  ala  A  100  ala  A  110  1_555
 sheet_1  strand_f  ala  A  120  ala  A  130  1_555
 sheet_1  strand_g  ala  A  140  ala  A  150  1_555
 sheet_1  strand_h  ala  A  160  ala  A  170  1_555
```

*Example 2 – five stranded mixed-sense sheet with one two-piece strand.*

```
loop_
_struct_sheet_range.sheet_id
_struct_sheet_range.id
_struct_sheet_range.beg_label_comp_id
_struct_sheet_range.beg_label_asym_id
_struct_sheet_range.beg_label_seq_id
_struct_sheet_range.end_label_comp_id
_struct_sheet_range.end_label_asym_id
_struct_sheet_range.end_label_seq_id
_struct_sheet_range.symmetry
 sheet_2  strand_a   ala  A  10  ala  A  18  1_555
 sheet_2  strand_b   ala  A 110  ala  A 119  1_555
 sheet_2  strand_c   ala  A  30  ala  A  41  1_555
 sheet_2  strand_d1  ala  A  50  ala  A  52  1_555
 sheet_2  strand_d2  ala  A  90  ala  A  97  1_555
 sheet_2  strand_e   ala  A  70  ala  A  80  1_555
```

**_struct_sheet_range.beg_auth_asym_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_sheet_range.beg_auth_comp_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_sheet_range.beg_auth_seq_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_struct_sheet_range.beg_label_asym_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_struct_asym.id** in the STRUCT_ASYM category.

* **_struct_sheet_range.beg_label_comp_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

* **_struct_sheet_range.beg_label_seq_id**
A component of the identifier for the residue at which the $\beta$-sheet range begins. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

**_struct_sheet_range.end_auth_asym_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_sheet_range.end_auth_comp_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_sheet_range.end_auth_seq_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

* **_struct_sheet_range.end_label_asym_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_struct_asym.id** in the STRUCT_ASYM category.

* **_struct_sheet_range.end_label_comp_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_chem_comp.id** in the CHEM_COMP category.

* **_struct_sheet_range.end_label_seq_id**
A component of the identifier for the residue at which the $\beta$-sheet range ends. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

* **_struct_sheet_range.id** (*code*)
The value of **_struct_sheet_range.id** must uniquely identify a range in a given sheet in the STRUCT_SHEET_RANGE list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*
***_struct_sheet_hbond.range_id_1***,
***_struct_sheet_hbond.range_id_2***,
***_struct_sheet_order.range_id_1***,
***_struct_sheet_order.range_id_2***,
***_struct_sheet_topology.range_id_1***,
***_struct_sheet_topology.range_id_2***. **[struct_sheet_range]**

* **_struct_sheet_range.sheet_id**
This data item is a pointer to **_struct_sheet.id** in the STRUCT_SHEET category.

**_struct_sheet_range.symmetry** (*symop*)
Describes the symmetry operation that should be applied to the residues delimited by the start and end designators in order to generate the appropriate strand in this sheet.
**[struct_sheet_range]**

## STRUCT_SHEET_TOPOLOGY

Data items in the STRUCT_SHEET_TOPOLOGY category record details about the topology of the residue ranges that form a $\beta$-sheet. All topology links are pairwise and the specified pairs are assumed to be successive in the amino-acid sequence. These data items are useful in describing various simple and complex folds, but they become inadequate when the strands in the sheet come from more than one chain. The STRUCT_SHEET_ORDER data items can be used to describe single- and multiple-chain-containing sheets.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_sheet_topology.sheet_id**
**_struct_sheet_topology.range_id_1**
**_struct_sheet_topology.range_id_2**

*Example 1 – simple beta-barrel.*

```
loop_
_struct_sheet_topology.sheet_id
_struct_sheet_topology.range_id_1
_struct_sheet_topology.range_id_2
_struct_sheet_topology.offset
_struct_sheet_topology.sense
 sheet_1  strand_a  strand_b  +1  parallel
 sheet_1  strand_b  strand_c  +1  parallel
 sheet_1  strand_c  strand_d  +1  parallel
 sheet_1  strand_d  strand_e  +1  parallel
 sheet_1  strand_e  strand_f  +1  parallel
 sheet_1  strand_f  strand_g  +1  parallel
 sheet_1  strand_g  strand_h  +1  parallel
 sheet_1  strand_h  strand_a  +1  parallel
```

*Example 2 – five stranded mixed-sense sheet with one two-piece strand.*

```
loop_
_struct_sheet_topology.sheet_id
_struct_sheet_topology.range_id_1
_struct_sheet_topology.range_id_2
_struct_sheet_topology.offset
_struct_sheet_topology.sense
 sheet_2  strand_a   strand_c    +2 anti-parallel
 sheet_2  strand_c   strand_d1   +1 anti-parallel
 sheet_2  strand_d1  strand_e    +1 anti-parallel
 sheet_2  strand_e   strand_d2   -1 anti-parallel
 sheet_2  strand_d2  strand_b    -2 anti-parallel
```

**_struct_sheet_topology.offset** (*int*)
Designates the relative position in the sheet, plus or minus, of the second residue range to the first.

[struct_sheet_topology]

***_struct_sheet_topology.range_id_1**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

***_struct_sheet_topology.range_id_2**
This data item is a pointer to **_struct_sheet_range.id** in the STRUCT_SHEET_RANGE category.

**_struct_sheet_topology.sense** (*ucode*)
A flag to indicate whether the two designated residue ranges are parallel or antiparallel to one another.

The data value must be one of the following:

parallel
anti-parallel

[struct_sheet_topology]

***_struct_sheet_topology.sheet_id**
This data item is a pointer to **_struct_sheet.id** in the STRUCT_SHEET category.

## STRUCT_SITE

Data items in the STRUCT_SITE category record details about portions of the structure that contribute to structurally relevant sites (*e.g.* active sites, substrate-binding subsites, metal-coordination sites).

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_site.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_site.id
_struct_site.details
 'P2 site C'
; residues with a contact < 3.7 \%A to an atom in the P2
  moiety of the inhibitor in the conformation with
     _struct_asym.id = C
;
 'P2 site D'
; residues with a contact < 3.7 \%A to an atom in the P1
  moiety of the inhibitor in the conformation with
     _struct_asym.id = D)
;
```

**_struct_site.details** (*text*)
A description of special aspects of the site.

[struct_site]

***_struct_site.id** (*line*)
The value of **_struct_site.id** must uniquely identify a record in the STRUCT_SITE list. Note that this item need not be a number; it can be any unique identifier.

*The following item(s) have an equivalent role in their respective categories:*
***_struct_site_gen.site_id***,
***_struct_site_keywords.site_id***,
***_struct_site_view.site_id***.

[struct_site]

## STRUCT_SITE_GEN

Data items in the STRUCT_SITE_GEN category record details about the generation of portions of the structure that contribute to structurally relevant sites.

Category group(s): **inclusive_group**
**struct_group**
Category key(s): **_struct_site_gen.id**
**_struct_site_gen.site_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_site_gen.id
_struct_site_gen.site_id
_struct_site_gen.label_comp_id
_struct_site_gen.label_asym_id
_struct_site_gen.label_seq_id
_struct_site_gen.symmetry
_struct_site_gen.details
  1  1  VAL  A   32  1_555  .
  2  1  ILE  A   47  1_555  .
  3  1  VAL  A   82  1_555  .
  4  1  ILE  A   84  1_555  .
  5  2  VAL  B  232  1_555  .
  6  2  ILE  B  247  1_555  .
  7  2  VAL  B  282  1_555  .
  8  2  ILE  B  284  1_555  .
```

**_struct_site_gen.auth_asym_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_asym_id** in the ATOM_SITE category.

**_struct_site_gen.auth_atom_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_atom_id** in the ATOM_SITE category.

**_struct_site_gen.auth_comp_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_comp_id** in the ATOM_SITE category.

**_struct_site_gen.auth_seq_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.auth_seq_id** in the ATOM_SITE category.

**_struct_site_gen.details** (*text*)
A description of special aspects of the symmetry generation of this portion of the structural site.

Example:
```
; The zinc atom lies on a special position; application of
symmetry elements to generate  the insulin hexamer will
generate excess zinc atoms, which must be removed by hand.
;
```
**[struct_site_gen]**

***_struct_site_gen.id** (*line*)
The value of **_struct_site_gen.id** must uniquely identify a record in the STRUCT_SITE_GEN list. Note that this item need not be a number; it can be any unique identifier.

**[struct_site_gen]**

***_struct_site_gen.label_alt_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_sites_alt.id** in the ATOM_SITES_ALT category.

***_struct_site_gen.label_asym_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_asym_id** in the ATOM_SITE category.

***_struct_site_gen.label_atom_id**
A component of the identifier for participants in the site. This data item is a pointer to **_chem_comp_atom.atom_id** in the CHEM_COMP_ATOM category.

***_struct_site_gen.label_comp_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_comp_id** in the ATOM_SITE category.

***_struct_site_gen.label_seq_id**
A component of the identifier for participants in the site. This data item is a pointer to **_atom_site.label_seq_id** in the ATOM_SITE category.

***_struct_site_gen.site_id**
This data item is a pointer to **_struct_site.id** in the STRUCT_SITE category.

**_struct_site_gen.symmetry** (*symop*)
Describes the symmetry operation that should be applied to the atom set specified by **_struct_site_gen.label*** to generate a portion of the site.

Examples: '`.`' (no symmetry or translation to site), '`4`' (4th symmetry operation applied), '`7_645`' (7th symmetry position: $+a$ on $x$, $-b$ on $y$). **[struct_site_gen]**

## STRUCT_SITE_KEYWORDS

Data items in the STRUCT_SITE_KEYWORDS category record keywords describing the site.

Category group(s): **inclusive_group**, **struct_group**
Category key(s): **_struct_site_keywords.site_id**, **_struct_site_keywords.text**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_struct_site_keywords.site_id
_struct_site_keywords.text
 'P2 site C'  'binding site'
 'P2 site C'  'binding pocket'
 'P2 site C'  'P2 site'
 'P2 site C'  'P2 pocket'
 'P2 site D'  'binding site'
 'P2 site D'  'binding pocket'
 'P2 site D'  'P2 site'
 'P2 site D'  'P2 pocket'
```

***_struct_site_keywords.site_id**
This data item is a pointer to **_struct_site.id** in the STRUCT_SITE category.

***_struct_site_keywords.text** (*text*)
Keywords describing this site.

Examples: '`active site`', '`binding pocket`', '`Ca coordination`'.
**[struct_site_keywords]**

## STRUCT_SITE_VIEW

Data items in the STRUCT_SITE_VIEW category record details about how to draw and annotate an informative view of the site.

Category group(s): **inclusive_group**, **struct_group**
Category key(s): **_struct_site_view.id**

*Example 1 – based on NDB structure GDL001 by Coll, Aymami, Van Der Marel, Van Boom, Rich & Wang [Biochemistry (1989), **28**, 310–320].*

```
_struct_site_view.id                    1
_struct_site_view.rot_matrix[1][1]     0.132
_struct_site_view.rot_matrix[1][2]     0.922
_struct_site_view.rot_matrix[1][3]    -0.363
_struct_site_view.rot_matrix[2][1]     0.131
_struct_site_view.rot_matrix[2][2]    -0.380
_struct_site_view.rot_matrix[2][3]    -0.916
_struct_site_view.rot_matrix[3][1]    -0.982
_struct_site_view.rot_matrix[3][2]     0.073
_struct_site_view.rot_matrix[3][3]    -0.172
_struct_site_view.details
; This view highlights the site of ATAT-Netropsin
  interaction.
;
```

**_struct_site_view.details** (*text*)
A description of special aspects of this view of the site. This data item can be used as a figure legend.

Example:
```
; The active site has been oriented with the specificity
pocket on the right and the active site machinery on the left.
;
```
**[struct_site_view]**

***_struct_site_view.id** (*line*)
The value of **_struct_site_view.id** must uniquely identify a record in the STRUCT_SITE_VIEW list. Note that this item need not be a number; it can be any unique identifier.

Examples: '`Figure 1`', '`unliganded enzyme`', '`view down enzyme active site`'. **[struct_site_view]**

**_struct_site_view.rot_matrix[1][1]** (*float*)
The [1][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[1][2]** (*float*)
The [1][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[1][3]** (*float*)
The [1][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[2][1]** (*float*)
The [2][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[2][2]** (*float*)
The [2][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[2][3]** (*float*)
The [2][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[3][1]** (*float*)
The [3][1] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[3][2]** (*float*)
The [3][2] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

**_struct_site_view.rot_matrix[3][3]** (*float*)
The [3][3] element of the matrix used to rotate the subset of the Cartesian coordinates in the ATOM_SITE category identified in the STRUCT_SITE_GEN category to an orientation useful for visualizing the site. The conventions used in the rotation are described in **_struct_site_view.details**.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}_{\text{reoriented Cartesian}} = \begin{pmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{\text{Cartesian}} .$$

**[struct_site_view]**

* **_struct_site_view.site_id**
This data item is a pointer to **_struct_site.id** in the STRUCT_SITE category.

## SYMMETRY

Data items in the SYMMETRY category record details about the space-group symmetry.

Category group(s): **inclusive_group**
**symmetry_group**
Category key(s): **_symmetry.entry_id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
_symmetry.entry_id                      '5HVP'
_symmetry.cell_setting                  orthorhombic
_symmetry.Int_Tables_number             18
_symmetry.space_group_name_H-M          'P 21 21 2'
```

**_symmetry.cell_setting** (*ucode*)
***_symmetry_cell_setting*** (*cif_core.dic 2.0.1*)
The cell settings for this space-group symmetry.
The data value must be one of the following:
triclinic
monoclinic
orthorhombic
tetragonal
rhombohedral
trigonal
hexagonal
cubic
**[symmetry]**

* **_symmetry.entry_id**
This data item is a pointer to **_entry.id** in the ENTRY category.

**_symmetry.Int_Tables_number** (*int*)
***_symmetry_Int_Tables_number*** (*cif_core.dic 2.0.1*)
Space-group number from *International Tables for Crystallography* Vol. A (2002).
**[symmetry]**

**_symmetry.space_group_name_H-M** (*line*)
***_symmetry_space_group_name_H-M*** (*cif_core.dic 2.0.1*)
Hermann–Mauguin space-group symbol. Note that the Hermann–Mauguin symbol does not necessarily contain complete information about the symmetry and the space-group origin. If used, always supply the *full* symbol from *International Tables for Crystallography* Vol. A (2002) and indicate the origin and the setting if it is not implicit. If there is any doubt that the equivalent positions can be uniquely deduced from this symbol, specify the **_symmetry_equiv.pos_as_xyz** or **_symmetry.space_group_name_Hall** data items as well. Leave spaces between symbols referring to different axes.
Examples: 'P 1 21/m 1', 'P 2/n 2/n 2/n (origin at -1)', 'R -3 2/m'.
**[symmetry]**

**_symmetry.space_group_name_Hall** (*line*)
***_symmetry_space_group_name_Hall*** (*cif_core.dic 2.0.1*)
Space-group symbol as described by Hall (1981). This symbol gives the space-group setting explicitly. Leave spaces between the separate components of the symbol.

Reference: Hall, S. R. (1981). *Acta Cryst.* A**37**, 517–525; erratum (1981), A**37**, 921.
Examples: '-P 2ac 2n', '-R 3 2"', 'P 61 2 2 (0 0 -1)'. **[symmetry]**

**SYMMETRY_EQUIV**

Data items in the SYMMETRY_EQUIV category list the symmetry-equivalent positions for the space group.
Category group(s): **inclusive_group**
**symmetry_group**
Category key(s): **_symmetry_equiv.id**

*Example 1 – based on PDB entry 5HVP and laboratory records for the structure corresponding to PDB entry 5HVP.*

```
loop_
_symmetry_equiv.id
_symmetry_equiv.pos_as_xyz
  1  '+x,+y,+z'
  2  '-x,-y,z'
  3  '1/2+x,1/2-y,-z'
  4  '1/2-x,1/2+y,-z'
```

* **_symmetry_equiv.id** (*code*)
***_symmetry_equiv_pos_site_id*** (*cif_core.dic 2.0.1*)
The value of **_symmetry_equiv.id** must uniquely identify a record in the SYMMETRY_EQUIV category. Note that this item need not be a number; it can be any unique identifier.
**[symmetry_equiv]**

**_symmetry_equiv.pos_as_xyz** (*line*)
***_symmetry_equiv_pos_as_xyz*** (*cif_core.dic 2.0.1*)
Symmetry-equivalent position in the '*xyz*' representation. Except for the space group *P*1, these data will be repeated in a loop. The format of the data item is as per *International Tables for Crystallography* Vol. A (2002). All equivalent positions should be entered, including those for lattice centring and a centre of symmetry, if present.
Example: '-y+x,-y,1/3+z'. **[symmetry_equiv]**

**VALENCE_PARAM**

Data items in the VALENCE_PARAM category define the parameters used for calculating bond valences from bond lengths. In addition to the parameters, a pointer is given to the reference (in VALENCE_REF) from which the bond-valence parameters were taken.
Category key(s): **_valence_param.atom_1**
**_valence_param.atom_1_valence**
**_valence_param.atom_2**
**_valence_param.atom_2_valence**

*Example 1 – a bond-valence parameter list with accompanying references.*

```
loop_
_valence_param.atom_1
_valence_param.atom_1_valence
_valence_param.atom_2
_valence_param.atom_2_valence
_valence_param.Ro
_valence_param.B
_valence_param.ref_id
_valence_param.details
  Cu 2 O -2 1.679 0.37 a .
  Cu 2 O -2 1.649 0.37 j .
  Cu 2 N -3 1.64  0.37 m '2-coordinate N'
  Cu 2 N -3 1.76  0.37 m '3-coordinate N'
loop_
_valence_ref.id
_valence_ref.reference
  a  'Brown & Altermatt (1985), Acta Cryst. B41, 244-247'
  j  'Liu & Thorp (1993), Inorg. Chem. 32, 4102-4205'
  m  'See, Krause & Strub (1998), Inorg. Chem. 37, 5369-5375'
```

* **_valence_param.atom_1** (*code*)
***_valence_param_atom_1*** (*cif_core.dic 2.3*)
The element symbol of the first atom forming the bond whose bond-valence parameters are given in this category.
**[valence_param]**

* **_valence_param.atom_1_valence** (*int*)
***_valence_param_atom_1_valence*** (*cif_core.dic 2.3*)
The valence (formal charge) of the first atom whose bond-valence parameters are given in this category.
**[valence_param]**

* **_valence_param.atom_2** (*code*)
***_valence_param_atom_2*** (*cif_core.dic 2.3*)
The element symbol of the second atom forming the bond whose bond-valence parameters are given in this category.
**[valence_param]**

*`_valence_param.atom_2_valence` (*int*)
`_valence_param_atom_2_valence` (*cif_core.dic 2.3*)
The valence (formal charge) of the second atom whose bond-valence parameters are given in this category.
`[valence_param]`

`_valence_param.B` (*float*)
`_valence_param_B` (*cif_core.dic 2.3*)
The bond-valence parameter $B$ used in the expression

$$s = \exp[(R_o - R)/B],$$

where $s$ is the valence of a bond of length $R$.
`[valence_param]`

`_valence_param.details` (*text*)
`_valence_param_details` (*cif_core.dic 2.3*)
Details of or comments on the bond-valence parameters.
`[valence_param]`

`_valence_param.id` (*code*)
`_valence_param_id` (*cif_core.dic 2.3*)
An identifier for the valence parameters of a bond between the given atoms.
`[valence_param]`

`_valence_param.ref_id` (*code*)
`_valence_param_ref_id` (*cif_core.dic 2.3*)
An identifier which links to the reference to the source from which the bond-valence parameters are taken. A child of `_valence_ref.id` which it must match.
`[valence_param]`

`_valence_param.Ro` (*float*)
`_valence_param_Ro` (*cif_core.dic 2.3*)
The bond-valence parameter $R_o$ used in the expression

$$s = \exp[(R_o - R)/B],$$

where $s$ is the valence of a bond of length $R$.
`[valence_param]`

## VALENCE_REF

Data items in the VALENCE_REF category list the references from which the bond-valence parameters have been taken.
Category key(s): `_valence_ref.id`

*`_valence_ref.id` (*code*)
`_valence_ref_id` (*cif_core.dic 2.3*)
An identifier for items in this category. Parent of `_valence_param.ref_id`, which must have the same value.
`[valence_ref]`

`_valence_ref.reference` (*text*)
`_valence_ref_reference` (*cif_core.dic 2.3*)
Literature reference from which the valence parameters identified by `_valence_param.id` were taken.
`[valence_ref]`