Format for Structure Factors

The deposited structure factor file should be the one that was used for the final refinement. This can either be in mmCIF, ASCII or mtz formats and should at least include h, k, l, F, SigmaF (and/or I and sigmaI) and test flags.

* Note: Deposition of structure factors is mandatory for the completion of an entry since February 1, 2008. 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.

_refln.F_meas_au	The measured value of the structure factor in arbitrary units
_refln.F_meas_sigma_au	The standard uncertainty (estimated standard deviation) of **_refln.F_meas_au** in arbitrary units
_refln.intensity_meas	The measured value of the intensity
_refln.intensity_sigma	The standard uncertainty (derived from measurement) of the intensity in the same units as **_refln.intensity_meas**
_refln.index_h	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.index_k	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.index_l	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.status	Classification of a reflection so as to indicate its status with respect to inclusion in the refinement and the calculation of R factors
_refln.pdbx_anom_difference	The amplitude difference of the Friedel pair D(hkl) = F(hkl) - F(-h-k-l)
_refln.pdbx_anom_difference_sigma	The standard deviation of the amplitude difference of the Friedel pair, D(hkl) = F(hkl) - F(-h-k-l)

Example 1:

```
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
```

Example 2:

```
data_rxxxxsf
#
_audit.revision_id      1_0
_audit.creation_date  ?
_audit.update_record    'Initial release'
#
#
_entry.id   rxxxxsf
#
#
_cell.entry_id     rxxxxsf
_cell.length_a             118.8600
_cell.length_b             155.0300
_cell.length_c             155.5400
_cell.angle_alpha           90.0000
_cell.angle_beta            90.0000
_cell.angle_gamma           90.0000
#
_symmetry.entry_id     rxxxxsf
_symmetry.Int_Tables_number        20
_symmetry.space_group_name_H-M     'C 2 2 21'
#
loop_
_symmetry_equiv.id
_symmetry_equiv.pos_as_xyz
1 'X,  Y,  Z'
2 '-X,  -Y,  Z+1/2'
3 'X,  -Y,  -Z'
4 '-X,  Y,  -Z+1/2'
5 'X+1/2,  Y+1/2,  Z'
```

```
6 '-X+1/2,  -Y+1/2,  Z+1/2'
7 'X+1/2,  -Y+1/2,  -Z'
8 '-X+1/2,  Y+1/2,  -Z+1/2'
#
_reflns.entry_id     rxxxxsf
_reflns.d_resolution_high          2.598
_reflns.d_resolution_low         47.140
_reflns.limit_h_max         45
_reflns.limit_h_min          0
_reflns.limit_k_max         59
_reflns.limit_k_min          0
_reflns.limit_l_max         59
_reflns.limit_l_min          0
_reflns.number_all        44453
_reflns.number_obs        44453
#
_diffrn_radiation_wavelength.id     1
#
_exptl_crystal.id     1
#
_reflns_scale.group_code     1
#
loop_
_refln.wavelength_id
_refln.crystal_id
_refln.scale_group_code
_refln.index_h
_refln.index_k
_refln.index_l
_refln.status
_refln.F_meas_au
_refln.F_meas_sigma_au
_refln.F_calc
_refln.phase_calc
_refln.fom
_refln.pdbx_HL_A_iso
_refln.pdbx_HL_B_iso
_refln.pdbx_HL_C_iso
_refln.pdbx_HL_D_iso
1 1 1    0    0    6 o   299.0    6.4   1306.2   0.0    0.32  0.33
0    0.00    0.00
1 1 1    0    0   10 o   726.8   15.0   1756.7   180.0  0.99  2.86
0    0.00    0.00
...
#END OF REFLECTIONS
```

Example 3:

```
data_rxxxxsf
#
_audit.revision_id      1_0
_audit.creation_date  ?
_audit.update_record    'Initial release'
#
#This file contains two data sets. The first data set is used for refinement.
#The second data set is used for phasing.
#
_entry.id   rxxxxsf
#
#
_cell.entry_id     rxxxxsf
_cell.length_a             108.7420
_cell.length_b              61.6790
_cell.length_c              71.6520
_cell.angle_alpha           90.0000
_cell.angle_beta            97.1510
_cell.angle_gamma           90.0000
#
_symmetry.entry_id     rxxxxsf
_symmetry.Int_Tables_number         5
_symmetry.space_group_name_H-M     'C 1 2 1'
#
loop_
_symmetry_equiv.id
_symmetry_equiv.pos_as_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'
#
_reflns.entry_id     rxxxxsf
_reflns.d_resolution_high          2.148
_reflns.d_resolution_low         70.711
_reflns.limit_h_max         50
_reflns.limit_h_min        -50
_reflns.limit_k_max         28
_reflns.limit_k_min          0
_reflns.limit_l_max         33
_reflns.limit_l_min          0
_reflns.number_all        25739
_reflns.number_obs        25471
#
_diffrn_radiation_wavelength.id     1
#
_exptl_crystal.id     1
#
_reflns_scale.group_code     1
#
loop_
_refln.wavelength_id
_refln.crystal_id
_refln.scale_group_code
```

```
_refln.index_h
_refln.index_k
_refln.index_l
_refln.status
_refln.F_meas_au
_refln.F_meas_sigma_au
1 1 1     -50    0    1 x         ?      ?
1 1 1      49    5    1 o      37.7    9.4
1 1 1      50    0    0 x         ?      ?
...
#END

data_rxxxxAsf
#
#This is second data set for phasing.
#
#
#
loop_
_cell.entry_id
_cell.CCP4_wavelength_id
_cell.CCP4_crystal_id
_cell.length_a
_cell.length_b
_cell.length_c
_cell.angle_alpha
_cell.angle_beta
_cell.angle_gamma
PHASE  1  1  108.7420  61.6790  71.6520  90.0000  97.1510  90.0000
PHASE  2  1  108.7420  61.6790  71.6520  90.0000  97.1510  90.0000
PHASE  3  1  108.7420  61.6790  71.6520  90.0000  97.1510  90.0000
PHASE  4  1  108.7420  61.6790  71.6520  90.0000  97.1510  90.0000
#
_symmetry.entry_id     PHASE
_symmetry.Int_Tables_number        5
_symmetry.space_group_name_H-M    'C 1 2 1'
#
loop_
_symmetry_equiv.id
_symmetry_equiv.pos_as_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'
#
loop_
_reflns.entry_id
_reflns.CCP4_wavelength_id
_reflns.CCP4_crystal_id
_reflns.d_resolution_high
_reflns.d_resolution_low
_reflns.limit_h_max
_reflns.limit_h_min
_reflns.limit_k_max
_reflns.limit_k_min
_reflns.limit_l_max
_reflns.limit_l_min
```

```
_reflns.number_all
_reflns.number_obs
PHASE  1  1    2.148   71.095    50   -50    28  0   33  0  25739  11565
PHASE  2  1    2.148   71.095    50   -50    28  0   33  0  25739  11895
PHASE  3  1    2.148   71.095    50   -50    28  0   33  0  25739  12000
PHASE  4  1    2.148   71.095    50   -50    28  0   33  0  25739  13346
#

loop_
_diffrn_radiation_wavelength.id
_diffrn_radiation_wavelength.CCP4_crystal_id
_diffrn_radiation_wavelength.wavelength
1  1      0.00000
2  1      0.00000
3  1      0.00000
4  1      0.00000
#
loop_
_exptl_crystal.id
1
#
_reflns_scale.group_code     1
#
loop_
_refln.wavelength_id
_refln.crystal_id
_refln.scale_group_code
_refln.index_h
_refln.index_k
_refln.index_l
_refln.status
_refln.F_meas_au
_refln.F_meas_sigma_au
_refln.pdbx_anom_difference
_refln.pdbx_anom_difference_sigma
1 1 1    -50    0    1 x        ?        ?        ?        ?
1 1 1    -50    0    2 x        ?        ?        ?        ?
...
#END OF REFLECTIONS
```

Example 4:

```
data_rxxxxsf
_entry.id   XXXX
_database_2.database_code   PDB
_database_2.database_id     XXXX
_audit.creation_date    'YYYY-MM-DD'

_cell.entry_id      XXXX
_cell.length_a      117.259
_cell.length_b      127.319
_cell.length_c      191.227
_cell.angle_alpha   90.00
_cell.angle_beta    90.29
_cell.angle_gamma   90.00
_cell.formula_units_Z   44
```

```
_symmetry.entry_id    XXXX
_symmetry.space_group_name_H-M  'P 1 21 1'

loop_
_symmetry_equiv.id
_symmetry_equiv.pos_as_xyz
       1  'X,Y,Z'
       2  '-X,Y+1/2,-Z'

_atom_sites.entry_id     XXXX
_atom_sites.fract_transf_matrix[1][1]     0.008528
_atom_sites.fract_transf_matrix[1][2]     0.000000
_atom_sites.fract_transf_matrix[1][3]     0.000043
_atom_sites.fract_transf_matrix[2][1]     0.000000
_atom_sites.fract_transf_matrix[2][2]     0.007854
_atom_sites.fract_transf_matrix[2][3]     0.000000
_atom_sites.fract_transf_matrix[3][1]     0.000000
_atom_sites.fract_transf_matrix[3][2]     0.000000
_atom_sites.fract_transf_matrix[3][3]     0.005229

_atom_sites.fract_transf_vector[1]         0.00000
_atom_sites.fract_transf_vector[2]         0.00000
_atom_sites.fract_transf_vector[3]         0.00000


_reflns.entry_id     XXXX
_reflns_scale.group_code 1
_exptl_crystal.id  1

_diffrn_radiation_wavelength.id 1
_diffrn_radiation_wavelength.wavelength 1.5418
_reflns.d_resolution_high          2.700
_reflns.d_resolution_low        182.574
_reflns.number_all       149457

loop_
_refln.wavelength_id
_refln.crystal_id
_refln.scale_group_code
_refln.index_h
_refln.index_k
_refln.index_l
_refln.status
_refln.F_meas_au
_refln.F_meas_sigma_au
…
#END OF REFLECTIONS
```