checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmwmsv3-130_f56_pydisulph_sq

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: dmwmsv3-130_f56_pydisulph_sq

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Bond precision:   C-C = 0.0034 A             Wavelength=0.68890

Cell:           a=32.81236(7)     b=30.21497(6)        c=40.09564(8)
                alpha=90          beta=96.3312(2)      gamma=90
Temperature:    100 K

                Calculated                  Reported
Volume          39509.35(14)                39509.35(10)
Space group     C 2/c                       C 1 2/c 1
Hall group      -C 2yc                      -C 2yc
                C336 H264 Co8 N72,          C336 H264 Co8 N72,
Moiety formula  0.554(C10 H8 N2 S2), B2     0.55(C10 H8 N2 S2), 14(B
                F5, 14(B F4), 2.446(        F4), B2 F5, 2.45(C
                C343.98 H278.22 B16 Co8     C380.04 H422.24 B16 Co8
Sum formula     F61 N73.11 O2.45 S1.11 [+   F64 N73.12 O38.44 S1.12
                solvent]
Mr              7314.00                     8525.63
Dx,g cm-3       1.230                       1.433
Z               4                           4
Mu (mm-1)       0.385                       0.411
F000            14944.7                     17647.0
F000'           14962.77
h,k,lmax        47,43,58                    47,43,58
Nref            62996                       62848
Tmin,Tmax                                   0.986,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.986 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.998          Theta(max)= 29.947

R(reflections)= 0.0672( 42312)     wR2(reflections)= 0.2358( 62848)

S = 1.098                 Npar= 2425
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The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F92   0.110 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F52   0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F72   0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   F82   0.122 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   92 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....   5 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   5 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..   1 Check

Alert level G
FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum: C380.0400 H422.2400 B16 Co8 F
           Atom count from _chemical_formula_moiety:C343.95 H278.2 B16 Co8 F61 N7
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C380.0400 H422.2400 B16 Co8 F64
           Atom count from the _atom_site data: C343.9842 H278.2151 B16 Co8 F61
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
             not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   4
           From the CIF: _chemical_formula_sum C380.04 H422.24 B16 Co8 F64 N73.12
           TEST: Compare cell contents of formula and atom_site data

           atom   Z*formula cif sites diff
           C   1520.16   1375.94   144.22
           H   1688.96   1112.86   576.10
           B   64.00   64.00   0.00
           Co   32.00   32.00   0.00
           F   256.00   244.00   12.00
           N   292.48   292.43   0.05
           O   153.76   9.78   143.98
           S   4.48   4.43   0.05
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   247 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   270 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT014_ALERT_1_G N.O.K.   _shelx_fab_checksum Found in CIF ......   Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.14 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.68890 Ang.
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing .... 0.00006 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing .... 0.00008 Ang.
PLAT145_ALERT_4_G s.u. on beta   Small or Missing ....   0.0002 Degree
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...   4 Units
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report

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PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records        36 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B11 Check
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B21 Check
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B31 Check
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B41 Check
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B51 Check
PLAT244_ALERT_4_G Low     Solvent Ueq as Compared to Neighbors of      B71 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F62        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F63        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F64        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F65        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B61        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F82        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F83        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F84        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F85        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B81        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O41S       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42S       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41S       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42A       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42B       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42C       Constrained at      0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13  )      100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )     6.09 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )     2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 11  )     2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )     4.34 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H23A     ..H15G     .     2.00 Ang.
                                    3/2-x,1/2-y,2-z  =     7_657 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H53C     ..H25G     .     2.07 Ang.
                                    3/2-x,1/2-y,2-z  =     7_657 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F75      ..C24G           2.93 Ang.
                                    x,y,z  =     1_555 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure     ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      509 Check
           B91  -F93  -B91     1.555   1.555   2.657        32.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #      510 Check
           B91  -F94  -B91     2.657   1.555   1.555        29.30 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       34 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        3 Note
           B2 F5
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        6 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        8 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        9 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       10 Note
           B F4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       11 Note
           B F4
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)     .     1.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co2       (II)     .     1.85 Info
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PLAT794_ALERT_5_G Tentative Bond Valency for Co3       (II)     .     1.85 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co4       (II)     .     1.83 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters     3 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............  6404 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed       ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).     2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600     56 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...    34 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     2 Info
PLAT984_ALERT_1_G The Co-f'=    0.3538 Deviates from the B&C-Value  0.3480 Check
PLAT984_ALERT_1_G The  S-f'=    0.1246 Deviates from the B&C-Value  0.1187 Check
PLAT985_ALERT_1_G The Co-f"=    0.9121 Deviates from the B&C-Value  0.9239 Check
PLAT985_ALERT_1_G The  S-f"=    0.1234 Deviates from the B&C-Value  0.1169 Check
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 84 ALERT level G = General information/check it is not something unexpected

 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 56 ALERT type 4 Improvement, methodology, query or suggestion
  5 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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