checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision: C-C = 0.0129 A Wavelength=1.54178

Cell: a=23.2078(19) b=23.5946(19) c=29.377(3)
alpha=90 beta=90 gamma=90

Temperature: 217 K

	Calculated	Reported
Volume	16086(2)	16086(2)
Space group	C m c a	C m c e
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	C106 H126 Co8 O42 S8, C H4 O, 2(H3 O) [+ solvent]	C106 H126 Co8 O42 S8, 0.5(C2 H8 O2), H6 O2
Sum formula	C107 H136 Co8 O45 S8 [+ solvent]	C107 H136 Co8 O45 S8
Mr	2870.08	2870.07
Dx,g cm-3	1.185	1.185
Z	4	4
Mu (mm-1)	7.817	7.817
F000	5928.0	5928.0
F000'	5880.48	
h,k,lmax	28,28,35	27,28,33
Nref	7614	7448
Tmin,Tmax	0.450,0.535	0.488,0.753
Tmin'	0.340	

Correction method= # Reported T Limits: Tmin=0.488 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 68.557

R(reflections)= 0.1131(3855)

wR2(reflections)= 0.3338(7448)

S = 1.165 Npar= 502

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

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.152
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.152 Report
PLAT082_ALERT_2_C High R1 Value ..................................    0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................    0.33 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O3       --C2       .     5.2 s.u.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O16      0.103 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O14      0.172 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O15      0.201 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01294 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -1.352 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       71 Report
               2  0  0,   4  0  0,   6  0  0,   0  2  0,  26 10  0,  14 24  0,
               1  1  1,  26 10  1,  15 23  1,  14 24  1,  13 25  1,  26 10  2,
              15 23  2,  14 24  2,   2  4  3,  15 23  3,  14 24  3,   4  0  4,
               3  3  4,  15 23  4,  14 24  4,   2  2  5,  15 23  5,  14 24  5,
              15 23  6,  15 23  7,  13 23 10,  12 24 10,  13 23 11,  13 23 12,
                  (   41 More Missing: see the .ckf listing file)
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         4 Note
               2  0  0,   0  2  0,   1  1  1,   3  3  4,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         2 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Co3      1.39 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Co2      1.03 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From O16     .      1.00 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.02Ang From O15     .      0.59 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.04Ang From O16     .      0.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21A      .     -0.45 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        16 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        34 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         6 Report
              H14C  H14A  H14B  H15A  H15B  H15C
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
              Calc: C106 H126 Co8 O42 S8, C H4 O, 2(H3 O)
              Rep.: C106 H126 Co8 O42 S8, 0.5(C2 H8 O2), H6 O2
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     22.00 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records        2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
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PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par     0.0100 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for SecondPar     0.0200 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par     0.0100 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for SecondPar     0.0200 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O9       --C21      .        5.8 s.u.
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             C21     H21A    H21B    H21C    O16     C28     O14     H14C
             O15
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15C       Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)        21% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)       100% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H6       ..H8AB     .       1.96 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H16      ..H19A     .       2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H23A     ..H14B     .       2.00 Ang.
                                                  1-x,y,z  =     11_655 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          6 Note
             H8AA    H8AB    H8AC    H9AA    H9AB    H9AC
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      15.60 Deg.
             H16A -O16  -H16A    1_555   1_555  11_655 ......     #  235 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      27.90 Deg.
             H14A -O14  -H14A    1_555   1_555  11_655 ......     #  268 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      31.40 Deg.
             H15A -O15  -H15C    1_555   1_555  11_655 ......     #  281 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          7 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        324 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         56 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
               2  2  5,   2  4  3,
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.          2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.          2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.832 Note
             Predicted wR2: Based on SigI**2 11.79 or SHELX Weight 28.64
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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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
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
49 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 21 ALERT type 2 Indicator that the structure model may be wrong or deficient
 17 ALERT type 3 Indicator that the structure quality may be low
 25 ALERT type 4 Improvement, methodology, query or suggestion
  3 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.

PLATON version of 04/06/2025; check.def file version of 30/05/2025

Datablock a - ellipsoid plot