checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PRG-II-57P

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: PRG-II-57P

Bond precision: C-C = 0.0044 A Wavelength=1.54184

Cell: a=9.9605(1) b=13.4937(1) c=22.5630(2)
alpha=88.176(1) beta=86.450(1) gamma=86.543(1)
Temperature: 100 K

	Calculated	Reported
Volume	3020.03(5)	3020.03(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H41 N7 O6, C32 H34 N2 O3 S [+ solvent]	C33 H41 N7 O6, C32 H34 N2 O3 S
Sum formula	C65 H75 N9 O9 S [+ solvent]	C65 H75 N9 O9 S
Mr	1158.40	1158.40
Dx,g cm-3	1.274	1.274
Z	2	2
Mu (mm-1)	1.004	1.004
F000	1232.0	1232.0
F000'	1236.25	
h,k,lmax	12,16,27	11,16,27
Nref	11517	11057
Tmin,Tmax	0.706,0.805	0.774,1.000
Tmin'	0.607	

Correction method= # Reported T Limits: Tmin=0.774 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta(max)= 70.282

R(reflections)= 0.0866(10413) wR2(reflections)= 0.2219(11057)

S = 1.041 Npar= 889

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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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.23 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       1.45 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O22      --C20      .        5.7 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O78 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00444 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N8       --H8B      .     Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C33 H41 N7 O6
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.566 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        216 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         44 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          6 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.06A   From O21            1.27 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         22 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         13 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          4 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S74A     --C73      .        6.9 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S74B     --C73      .       10.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O78      --C77A     .       14.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O78      --C77C     .       10.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of S74A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S74B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S74C       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O75A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O75B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O75C       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C76A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C77A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C76B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C76C       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C77B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C77C       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77B       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H73C       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73D       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73E       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H73F       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76C       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76D       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76E       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H76F       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77C       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77D       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77E       Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H77F       Constrained at        0.2 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        13% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        11% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H32A     ..H31C     .       2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H32B     ..H31D     .       2.12 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H72A     ..H73D     .       2.11 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H80      ..H77E     .       1.95 Ang.
                                                    x,y,z  =      1_555 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H32B     ..H29C     .       2.06 Ang.
                                                 -1-x,-1-y,-1-z  =      2_444 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H34A     ..H77D     .       2.04 Ang.
                                                  1+x,-1+y,z  =      1_645 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H41      ..H77D     .       1.85 Ang.
                                                  1+x,-1+y,z  =      1_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  S74B     ..C39              3.27 Ang.
                                                  -2-x,-y,-2-z  =      2_353 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C41      ..C77B             3.09 Ang.
                                                  1+x,-1+y,z  =      1_645 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         30 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....               3 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C32 H34 N2 O3 S
PLAT793_ALERT_4_G Model has Chirality at C7          (Centro SPGR)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       306 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        203 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.2 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          5 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
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
65 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
42 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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 13/07/2021; check.def file version of 13/07/2021

Datablock PRG-II-57P - ellipsoid plot