

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) DLM770_1

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: DLM770_1

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

Cell: a=15.2504(3) b=17.0326(4) c=17.2393(3)
 alpha=106.910(2) beta=103.444(2) gamma=110.252(2)
Temperature: 100 K

	Calculated	Reported
Volume	3732.35(17)	3732.34(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H49 N7 O8, C32 H34 N2 O3 S [+ solvent]	C70 H83 N9 O11 S
Sum formula	C70 H83 N9 O11 S [+ solvent]	C70 H83 N9 O11 S
Mr	1258.51	1258.51
Dx, g cm ⁻³	1.120	1.120
Z	2	2
Mu (mm ⁻¹)	0.103	0.103
F000	1340.0	1340.0
F000'	1340.82	
h, k, lmax	22, 25, 25	22, 25, 25
Nref	26543	23034
Tmin, Tmax	0.970, 0.985	0.819, 1.000
Tmin'	0.953	

Correction method= # Reported T Limits: Tmin=0.819 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.868

Theta(max)= 32.289

R(reflections)= 0.0616(17323)

wR2(reflections)= 0.1698(23034)

S = 1.025

Npar= 915

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

PLAT213_ALERT_2_C	Atom C33A	has ADP max/min Ratio	3.2	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		4.852	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		6	Note

● Alert level G

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 ...		10	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		1	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please	Check
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...		2	Units
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002	Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		21	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for 032 --C33A .		7.6	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C33	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C34	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C35	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C37	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C39	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C41	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C42	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C33A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C34A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C35A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C37A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C39A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C40A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C41A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C42A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33D	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37D	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38B	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39D	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40D	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41A	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41B	Constrained at	0.75	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H42C	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42D	Constrained at	0.75	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H39B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42B	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		19%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H25 ..H33A .		2.02	Ang.
	x,y,z =	1_555		Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H25 ..H33B .		2.14	Ang.
	x,y,z =	1_555		Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H45 ..H42A .		2.10	Ang.
	x,y,z =	1_555		Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H45 ..H42B .		2.08	Ang.
	x,y,z =	1_555		Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H111 ..H35C .		1.93	Ang.
	x,y,z =	1_555		Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		!	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		75	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		3501	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		15	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 83 **ALERT level G** = General information/check it is not something unexpected

3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 12 **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
 66 **ALERT type 4** Improvement, methodology, query or suggestion
 1 **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.

