

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0044 Å Wavelength=0.71073

Cell: a=7.8563 (8) b=9.2517 (10) c=21.803 (2)
 alpha=95.923 (3) beta=98.136 (2) gamma=96.538 (3)
Temperature: 298 K

	Calculated	Reported
Volume	1547.1 (3)	1547.1 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H31 N5 O [+ solvent]	C36 H31 N5 O
Sum formula	C36 H31 N5 O [+ solvent]	C36 H31 N5 O
Mr	549.66	549.66
Dx, g cm ⁻³	1.180	1.180
Z	2	2
Mu (mm ⁻¹)	0.073	0.073
F000	580.0	580.0
F000'	580.20	
h, k, lmax	10, 12, 28	10, 11, 28
Nref	7095	7053
Tmin, Tmax	0.982, 0.999	0.686, 0.746
Tmin'	0.960	

Correction method= # Reported T Limits: Tmin=0.686 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.490

R(reflections)= 0.0696 (3472)	wR2(reflections)=
S = 1.026	0.2094 (7053)
Npar= 380	

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 B

PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note



Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49%	Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.65	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.72	eA-3
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C16 --C17 .	6.0	s.u.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0044	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C36 H31 N5 O		
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	33.051	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	6.240	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.643	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	11	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	128	A**3
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).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	28	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

