

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2840abs

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: AX2840abs

Bond precision:	C-C = 0.0022 A	Wavelength=0.71073	
Cell:	a=9.8461 (7)	b=24.1926 (16)	c=11.2997 (7)
	alpha=90	beta=97.556 (2)	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	2668.3(3)	2668.2(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H32 N6 O8	C26 H32 N6 O8
Sum formula	C26 H32 N6 O8	C26 H32 N6 O8
Mr	556.58	556.57
Dx, g cm-3	1.385	1.385
Z	4	4
Mu (mm-1)	0.104	0.104
F000	1176.0	1176.0
F000'	1176.59	
h, k, lmax	12, 29, 13	12, 29, 13
Nref	5236	5236
Tmin, Tmax	0.984, 0.989	0.603, 0.746
Tmin'	0.960	

Correction method= # Reported T Limits: Tmin=0.603 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta (max)= 26.000

R(reflections)= 0.0396(3972)	wR2(reflections)= 0.1071(5236)
S = 1.013	Npar= 383

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...				-0.129	Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0010	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0010	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	5%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3 ..C3 .	3.17	Ang.
	1-x,1-y,1-z =	3_666	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*Sigma(I)	4	Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.728	Note
	Predicted wR2: Based on SigI**2 2.87 or SHELX Weight 10.56		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8	Info

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

- 1 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
6 ALERT type 3 Indicator that the structure quality may be low
1 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.

