

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2850abs

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: AX2850abs

Bond precision:	C-C = 0.0034 A	Wavelength=1.54178		
Cell:	a=8.7897 (5)	b=15.3948 (8)	c=21.7326 (12)	
	alpha=90	beta=90	gamma=90	
Temperature:	150 K			

	Calculated	Reported
Volume	2940.8(3)	2940.8(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C28 H40 N6 O8	C28 H40 N6 O8
Sum formula	C28 H40 N6 O8	C28 H40 N6 O8
Mr	588.66	588.66
Dx, g cm ⁻³	1.330	1.330
Z	4	4
Mu (mm ⁻¹)	0.818	0.818
F000	1256.0	1256.0
F000'	1260.10	
h, k, lmax	10, 18, 25	10, 18, 25
Nref	5201[2954]	5182
Tmin, Tmax	0.850, 0.886	0.498, 0.753
Tmin'	0.850	

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Correction method= # Reported T Limits: Tmin=0.498 Tmax=0.753
AbsCorr = MULTI-SCAN
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Data completeness= 1.75/1.00 Theta (max)= 66.564

R(reflections)= 0.0318(5138)	wR2(reflections)= 0.0839(5182)
S = 1.049	Npar= 387

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

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

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max.	(Positive) Residual Density	0.64 eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.8 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.1 Ratio
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	9 Report
	2 15 14, 0 3 24, 2 0 25, 0 1 25, 0 2 25, 0 3 25,		
	1 3 25, 0 4 25, 1 4 25,		



Alert level G

PLAT791_ALERT_4_G	Model has Chirality at C13	(Sohncke SpGr)	S Verify
PLAT791_ALERT_4_G	Model has Chirality at C21	(Sohncke SpGr)	S Verify
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		99% Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		4.599 Note
	Predicted wR2: Based on SigI**2 1.82 or SHELX Weight	8.00	
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
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
6 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

