

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2767abs2

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: AX2767abs2

Bond precision:	C-C = 0.0033 A	Wavelength=0.71073	
Cell:	a=27.446 (5)	b=11.970 (2)	c=18.952 (3)
	alpha=90	beta=107.682 (4)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	5932.1 (17)	5932.3 (18)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	2 (C24 H32 N6 O8), C4 H10 O, 2 (C24 H32 N6 O8), C4 H10 O, 2 (H2 O)	2 (C24 H32 N6 O8), C4 H10 O, 2 (H2 O)	
Sum formula	C52 H78 N12 O19	C52 H78 N12 O19	
Mr	1175.26	1175.26	
Dx, g cm-3	1.316	1.316	
Z	4	4	
Mu (mm-1)	0.101	0.101	
F000	2504.0	2504.0	
F000'	2505.30		
h, k, lmax	33, 14, 23	33, 14, 23	
Nref	11661	11659	
Tmin, Tmax	0.981, 0.984	0.687, 0.746	
Tmin'	0.968		

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta (max)= 25.999

R(reflections)= 0.0451 (8522)

wR2(reflections)=
0.1226 (11659)

S = 1.017

Npar= 782

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

PLAT430_ALERT_2_B Short Inter D...A Contact O15 ..N13 . 2.84 Ang.
-x,-1/2+y,1/2-z = 2_545 Check

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -0.677

Test value = -0.600

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.68 eA-3

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C62 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of O21 Check

PLAT411_ALERT_2_C Short Inter H...H Contact H41B ..H63A . 2.13 Ang.
-1+x,y,z = 1_455 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 5 Report

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT432_ALERT_2_G Short Inter X...Y Contact O5 ..C7 . 2.99 Ang.
1-x,1/2+y,1/2-z = 2_655 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O15 ..C35 . 2.77 Ang.
-x,-1/2+y,1/2-z = 2_545 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact O15 ..C34 . 2.94 Ang.
-x,-1/2+y,1/2-z = 2_545 Check

PLAT860_ALERT_3_G Number of Least-Squares Restraints 32 Note

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
1 0 0,

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
-10 3 1,

PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 5 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 5.857 Note

Predicted wR2: Based on SigI**2 2.09 or SHELX Weight 12.06

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

11 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
4 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 22/08/2024; check.def file version of 21/08/2024

