



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AX2917abs_a

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: AX2917abs_a

Bond precision:	C-C = 0.0086 Å	Wavelength=1.54178	
Cell:	a=14.5984 (3)	b=14.5984 (3)	c=17.1526 (4)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	3655.45 (17)	3655.45 (17)	
Space group	P 43 21 2	P 43 21 2	
Hall group	P 4nw 2abw	P 4nw 2abw	
Moiety formula	C34 H40 N8 O10, C0.49 H0.98 C10.97	C34 H40 N8 O10, C0.49 H0.98 C10.97	
Sum formula	C34.49 H40.98 C10.97 N8 O10	C34.49 H40.98 C10.97 N8 O10	
Mr	762.10	762.06	
Dx, g cm-3	1.385	1.385	
Z	4	4	
Mu (mm-1)	1.491	1.490	
F000	1601.8	1602.0	
F000'	1608.40		
h, k, lmax	17, 17, 20	17, 17, 20	
Nref	3239 [1905]	3238	
Tmin, Tmax	0.776, 0.817	0.515, 0.753	
Tmin'	0.704		

Correction method= # Reported T Limits: Tmin=0.515 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.70/1.00

Theta(max)= 66.583

R(reflections)= 0.0702(2974)

wR2(reflections)=
0.2099(3238)

S = 1.023

Npar= 289

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

PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms .	Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax <= 18)	6.59 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.21 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C13 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11	0.143 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00864 Ang.



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms	8 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0100 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	15% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2)	2.44 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C10 - C11 .	1.51 Ang.
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H7A ..H15D .	2.13 Ang.
	y,x,1-z = 7_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C15' .	3.01 Ang.
	1/2+y,1/2-x,1/4+z = 4_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 ..C15 .	3.01 Ang.
	1/2+y,1/2-x,1/4+z = 4_555 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit-Cell: Resd. #	2 Note
C0.49 H0.98 Cl0.97	
PLAT860_ALERT_3_G Number of Least-Squares Restraints	45 Note
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	81% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	1 Note
0 2 1,	
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	7.341 Note
Predicted wR2: Based on SigI**2 2.86 or SHELX Weight	20.52
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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

2 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
9 ALERT type 3 Indicator that the structure quality may be low
7 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

