



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ks1736

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: ks1736

Bond precision:	C-C = 0.0049 Å	Wavelength=0.71073
Cell:	a=12.5101 (4) alpha=90	b=7.7677 (2) beta=113.431 (3) c=14.8027 (5) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1319.83 (8)	1319.83 (8)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
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	1.401	1.401
Z	2	2
Mu (mm ⁻¹)	0.106	0.106
F000	588.0	588.0
F000'	588.30	
h, k, lmax	15, 9, 18	15, 9, 18
Nref	5201 [2804]	5149
Tmin, Tmax	0.985, 0.992	1.000, 1.000
Tmin'	0.981	

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.99

Theta(max)= 25.999

R(reflections)= 0.0387(4661)

wR2(reflections)=
0.1042(5149)

S = 1.009

Npar= 365

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.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.06	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.76	eA-3
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours		C22 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00489	Ang.



Alert level G

PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.300	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C5 .	2.93	Ang.
	1-x,1/2+y,1-z =	2_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C7 .	2.94	Ang.
	1-x,1/2+y,1-z =	2_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2 ..C2 .	2.96	Ang.
	1-x,1/2+y,1-z =	2_656	Check
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 with s.u.	0.30	Check
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	1.77	Note
	0 0 1,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
	-3 0 3,		
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	7.824	Note
	Predicted wR2: Based on SigI**2 1.33 or SHELX Weight 10.33		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..		! Note

- 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
12 **ALERT level G** = General information/check it is not something unexpected

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

Datablock ks1736 - ellipsoid plot

