



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0134 Å		Wavelength=1.54178
Cell:	a=15.0432 (9)	b=12.9768 (10)	c=19.2547 (12)
	alpha=90	beta=106.479 (4)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	3604.4 (4)	3604.4 (4)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C18 H34 N6 O2, 2 (C6 H2 N3 O7)	?	
Sum formula	C30 H38 N12 O16	C30 H38 N12 O16	
Mr	822.72	822.72	
Dx, g cm-3	1.516	1.516	
Z	4	4	
Mu (mm-1)	1.072	1.072	
F000	1720.0	1720.0	
F000'	1726.42		
h, k, lmax	15, 12, 19	15, 12, 19	
Nref	3764	3758	
Tmin, Tmax	0.898, 0.898	0.870, 0.900	
Tmin'	0.898		

Correction method= # Reported T Limits: Tmin=0.870 Tmax=0.900
AbsCorr = MULTISCAN

Data completeness= 0.998

Theta(max)= 50.421

R(reflections)= 0.1079(2757)

wR2(reflections)=
0.3003(3758)

S = 1.050

Npar= 524

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4999

Alert level B

PLAT088_ALERT_3_B	Poor Data / Parameter Ratio	7.17	Note
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	1.50	eA-3
PLAT234_ALERT_4_B	Large Hirshfeld Difference O4 --N7 .	0.26	Ang.
PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds	0.01342	Ang.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range of ...	2.667	Sigma
PLAT082_ALERT_2_C	High R1 Value	0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.30	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.55	Report
PLAT214_ALERT_2_C	Atom N7 (Anion/Solvent) ADP max/min Ratio	4.3	prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference O5 --N7 .	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N7 --C21 .	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N9 --C23 .	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21 --C22 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C22 --C23 .	0.25	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N7	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N9	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C22	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	3.2	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including 03	0.114	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	7.936	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.500	5	Report

3 0 1, -3 0 3, -4 0 4, 8 7 7, 7 6 8,

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
	H1 H6		
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	18.97	Why ?
PLAT432_ALERT_2_G	Short Inter X...Y Contact O11 ..C9 .	3.02	Ang.
	1-x,-y,1-z =	3_656	Check

PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	49%	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	4.16	Note
	-1 0 1,		
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
	-4 0 4,		
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	3.381	Note
	Predicted wR2: Based on SigI**2 8.88 or SHELX Weight 28.59		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_shelx
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT088_shelx
;
PROBLEM: Poor Data / Parameter Ratio ..... 7.17 Note
RESPONSE: ...
;
_vrf_PLAT097_shelx
;
PROBLEM: Large Reported Max. (Positive) Residual Density 1.50 eA-3
RESPONSE: ...
;
_vrf_PLAT234_shelx
;
PROBLEM: Large Hirshfeld Difference O4 --N7 . 0.26 Ang.
RESPONSE: ...
;
_vrf_PLAT340_shelx
;
```

PROBLEM: Low Bond Precision on C-C Bonds 0.01342 Ang.
RESPONSE: ...

;
end Validation Reply Form

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

duplicate check

No duplication found

Datablock shelx - ellipsoid plot

