



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ks1749_sq

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: ks1749_sq

Bond precision: C-C = 0.0097 Å

Wavelength=0.71073

Cell: a=9.5279 (6) b=12.7827 (9) c=17.7588 (13)
 alpha=94.807 (6) beta=96.335 (6) gamma=108.423 (5)
Temperature: 150 K

	Calculated	Reported
Volume	2023.3 (3)	2023.3 (2)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C40 H46 N8 O8 [+ solvent]	C40 H46 N8 O8
Sum formula	C40 H46 N8 O8 [+ solvent]	C40 H46 N8 O8
Mr	766.85	766.85
Dx, g cm ⁻³	1.259	1.259
Z	2	2
Mu (mm ⁻¹)	0.090	0.090
F000	812.0	812.0
F000'	812.37	
h, k, lmax	11, 15, 21	11, 15, 21
Nref	15914 [7957]	14183
Tmin, Tmax	0.988, 0.993	1.000, 1.000
Tmin'	0.975	

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = ?

Data completeness= 1.78/0.89

Theta(max)= 26.000

R(reflections)= 0.0563(10464)

wR2(reflections)=
0.1451(14183)

S = 1.016

Npar= 1033

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

PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O6	--H6O	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O28	--H28O	.	Please Check

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
 From the CIF: _refine_ls_abs_structure_Flack -0.600
 From the CIF: _refine_ls_abs_structure_Flack_su 0.700

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.5	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2	C	Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	4.8	Ratio
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C38	Check	
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C39	Check	
PLAT241_ALERT_2_C	High	MainResAtom	Ueq as Compared to Neighbours	C64	Check	
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C34	Check	
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C60	Check	
PLAT242_ALERT_2_C	Low	MainResAtom	Ueq as Compared to Neighbours	C63	Check	
PLAT331_ALERT_2_C	Small	Aver Phenyl C-C Dist	C34	--C39	.	1.37 Ang.
PLAT340_ALERT_3_C	Low	Bond Precision on C-C Bonds			0.00971	Ang.
PLAT352_ALERT_3_C	Short	N-H (X0.87,N1.01A)	N8	- H8N	.	0.74 Ang.
PLAT415_ALERT_2_C	Short	Inter D-H..H-X	H28O	..H76	.	2.09 Ang.
				-1+x,y,z =	1_455	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600		10	Report
	5 8 6,	5 9 6,	5 8 7,	5 7 8,	5 8 8,	5 6 9,
	5 7 9,	5 8 9,	5 6 10,	5 7 10,		
PLAT915_ALERT_3_C	No	Flack x Check Done: Low Friedel Pair Coverage			78	%

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or U(i,j)	Restrained non-H-Atoms	6	Report	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		4	Report	
	H6O	H8O	H26O	H28O	
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High	.	0.700	Report	
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report	
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0100	Report	
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O8	..C6	.	2.86 Ang.
			1+x,y,z =	1_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O26	..C41	.	2.77 Ang.
			-1+x,y,z =	1_455	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		163	A**3	
PLAT791_ALERT_4_G	Model has Chirality at C18	(Sohncke SpGr)	S	Verify	
PLAT791_ALERT_4_G	Model has Chirality at C32	(Sohncke SpGr)	S	Verify	

PLAT791_ALERT_4_G Model has Chirality at C58	(Sohncke SpGr)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C72	(Sohncke SpGr)	S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints		39 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed		! Info
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]=		1.69 Note
0 0 1,		
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	4 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .	0.20	Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		3 Note
-1 1 -2, -1 1 1, -1 0 -1,		
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.4 Low
PLAT960_ALERT_3_G Number of Intensities with I < - 2*Sigma(I)		3 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		6.482 Note
Predicted wR2: Based on SigI**2	2.24 or SHELX Weight	14.27 Note
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
 2 **ALERT level B** = A potentially serious problem, consider carefully
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 24 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 3 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 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

