



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CEC0498SQ

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: CEC0498SQ

Bond precision:	C-C = 0.0008 Å	Wavelength=0.71073
Cell:	a=13.1949 (15) alpha=90	b=12.6702 (14) beta=99.610 (5)
		c=9.8792 (11) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1628.5 (3)	1628.4 (3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H16 Cl2 N2 O3 [+ solvent]	C14 H16 Cl2 N2 O3
Sum formula	C14 H16 Cl2 N2 O3 [+ solvent]	C14 H16 Cl2 N2 O3
Mr	331.19	331.19
Dx, g cm ⁻³	1.351	1.351
Z	4	4
Mu (mm ⁻¹)	0.409	0.409
F000	688.0	688.0
F000'	689.46	
h, k, lmax	26, 25, 19	26, 25, 19
Nref	13728	13680
Tmin, Tmax	0.907, 0.980	0.900, 0.980
Tmin'	0.894	

Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.980
AbsCorr = NUMERICAL

Data completeness= 0.997 Theta(max)= 45.410

R(reflections)= 0.0332(10884) wR2(reflections)=
0.0998(13680)

S = 1.015 Npar= 210

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

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...	-0.214	Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
2 6 0, -5 7 1,		
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From N4 .	-0.51	eA-3

🟢 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	11	Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms	1	Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms H4	1	Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O13 --C7 .	5.4	s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	24%	Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	67	A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels H9'1 H9'2	2	Note
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SpGr)	R	Verify
PLAT793_ALERT_4_G Model has Chirality at C5 (Centro SpGr)	R	Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints	14	Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 1 0 0,	2.24	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	47	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 6 0, -5 7 1,	2	Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..	91.0	Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value Predicted wR2: Based on SigI**2 2.54 or SHELX Weight	3.938	Note
9.83		
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	12	Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by	2	Check
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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
26 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
4 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 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

