

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3Cl-decomposition

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: 3Cl-decomposition

Bond precision: C-C = 0.0086 Å

Wavelength=1.54178

Cell: a=7.4241(5) b=12.4935(9) c=20.8699(12)
 alpha=84.241(6) beta=83.819(5) gamma=83.303(6)
Temperature: 293 K

	Calculated	Reported
Volume	1903.8(2)	1903.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H39.19 Cl4.81 N2 O6, C42 H39.44 Cl4.56 N2 O6	2(C42 H39.19 Cl4.81 N2 O6)
Sum formula	C84 H78.63 Cl9.37 N4 O12	C84 H78.63 Cl9.37 N4 O12
Mr	1668.37	1668.30
Dx,g cm-3	1.455	1.455
Z	1	1
Mu (mm-1)	3.699	3.698
F000	866.0	866.0
F000'	871.54	
h,k,lmax	8,14,24	8,14,23
Nref	6117	5920
Tmin,Tmax	0.674,0.691	0.554,0.725
Tmin'	0.547	

Correction method= # Reported T Limits: Tmin=0.554 Tmax=0.725
AbsCorr = EMPIRICAL

Data completeness= 0.968

Theta(max)= 62.702

R(reflections)= 0.0919(3634)

wR2(reflections)= 0.2651(5920)

S = 1.027

Npar= 515

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

PLAT220_ALERT_2_B	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	6.8 Ratio
PLAT410_ALERT_2_B	Short Intra H...H Contact	H40A ..H46C	1.88 Ang.
PLAT936_ALERT_2_B	The Embedded .res File Includes a DAMP Command	.	500.0 Report

Alert level C

THETM01_ALERT_3_C	The value of sine(theta_max)/wavelength is less than 0.590		
	Calculated sin(theta_max)/wavelength = 0.5764		
PLAT018_ALERT_1_C	_diffrn_measured_fraction_theta_max .NE. *_full		! Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	8.2 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C35	--C37	0.18 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C36	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C37	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C40	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C42	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C46	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C39	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C45	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0086	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C38	- C40	1.42 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H31B ..H35A	1.96 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H30A ..H33A	1.95 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H42B ..H43A	1.95 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.063	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.788	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.576	195 Report

Alert level G

FORMU01_ALERT_1_G	There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.		
	Atom count from _chemical_formula_sum: C84 H78.62999 Cl9.37 N4 O12		
	Atom count from _chemical_formula_moiety: C84 H78.37999 Cl9.62 N4 O12		
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	16	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	8	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	13	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	4	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C33	--C43	6.7 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	23% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		22% Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O7AA	107.7	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2AA	108.2	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	11	Note

PLAT793_ALERT_4_G Model has Chirality at C35	(Centro SPGR)	S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints		105 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...		11 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		1 Info

0	ALERT level A	= Most likely a serious problem - resolve or explain
3	ALERT level B	= A potentially serious problem, consider carefully
24	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
22	ALERT level G	= General information/check it is not something unexpected
5	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
25	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
9	ALERT type 4	Improvement, methodology, query or suggestion
0	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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

