

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1_a_sq

Bond precision:	C-C = 0.0225 A	Wavelength=0.71073
Cell:	a=25.3747(16)	b=20.3378(15) c=17.3896(11)
	alpha=90	beta=90.087(2) gamma=90
Temperature:	200 K	
	Calculated	Reported
Volume	8974.2(10)	8974.2(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C45 H50 Ca Cl N20 O10, 5(C6 H5 N O3), C6 H4 N O3, Cl, H2 O [+ s	C45 H50 Ca Cl N20 O10, 5(C6 H5 N O3), C6 H4 N O3, H2 O
Sum formula	C81 H81 Ca Cl2 N26 O29 [+ solvent]	C81 H81 Ca Cl2 N26 O29
Mr	1993.70	1993.69
Dx, g cm-3	1.476	1.476
Z	4	4
Mu (mm-1)	0.226	0.226
F000	4140.0	4140.0
F000'	4144.12	
h, k, lmax	30, 24, 20	30, 24, 20
Nref	15803	15757
Tmin, Tmax	0.949, 0.960	0.668, 0.746
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.668 Tmax=0.746
AbsCorr = MULTII-SCAN

Data completeness= 0.997

Theta(max)= 24.997

R(reflections)= 0.1861(13234)

wR2(reflections)=
0.4430(15757)

S = 1.102

Npar= 1264

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

PLAT082_ALERT_2_B	High R1 Value	0.19	Report
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.44	Report
PLAT234_ALERT_4_B	Large Hirshfeld Difference N21 --C61 .	0.30	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference C60 --C61 .	0.26	Ang.
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of C60		Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of N21		Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of C61		Check
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds	0.02254	Ang.
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O17 --H17 .		Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O23 --H23 .		Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O26 --H26 .		Please Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O4 ..020 .	2.79	Ang.
	x,y,z =	1_555	Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O15 ..025 .	2.82	Ang.
	2-x,-y,-z =	3_755	Check

● Alert level C

PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for O20 .	6	Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference O5 --C3 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N17 --C17 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C14 --C15 .	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C42 --C43 .	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C55 --C56 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C70 --C71 .	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C70 --C75 .	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C73 --C74 .	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C68 --C69 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C77 --C78 .	0.19	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C14		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C43		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C72		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C65		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C63		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C15		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of N25		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of N24		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C70		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C73		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of N23		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C64		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C67		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C58		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C59		Check

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N26	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	2.3	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	2.9	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including 023	0.141	Check
PLAT309_ALERT_2_C	Single	Bonded Oxygen (C-O > 1.3 Ang)	020	Check
PLAT334_ALERT_2_C	Small	Aver. Benzene C-C Dist C64 -C69	1.37	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	7	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	237.56	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	1%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H20A ..H82B .	2.01	Ang.
	x,1/2-y,-1/2+z =	4_565	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H23 ..H43B .	1.84	Ang.
	x,1/2-y,-1/2+z =	4_565	Check
PLAT415_ALERT_2_G	Short Inter D-H..H-X H23 ..H43C .	1.95	Ang.
	x,1/2-y,-1/2+z =	4_565	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	191	A**3
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	9	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 39 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 17 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. 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.

