

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: I

Bond precision:	C-C = 0.0097 A	Wavelength=1.54178
Cell:	a=37.7211(9)	b=20.6072(5) c=21.3384(5)
	alpha=90	beta=90 gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	16586.9(7)	16586.9(7)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	2(C80 H78 N8 O16), 2(C79.70 H77.55 N8 O15.85), 10.186(C H Cl3),	11.59(C H Cl3), 4(C80 H78 N8 O16), H2O
Sum formula	C331.89 H323.59 Cl34.76 N32 O65	C331.89 H325.58 Cl34.75 N32 O65
Mr	7032.63	7034.32
Dx,g cm-3	1.408	1.408
Z	2	2
Mu (mm-1)	3.283	3.282
F000	7299.6	7303.0
F000'	7344.57	
h,k,lmax	45,24,25	45,23,25
Nref	30884[16586]	30115
Tmin,Tmax	0.854,0.906	0.635,0.753
Tmin'	0.697	

Correction method= MULTI-SCAN

Data completeness= 1.82/0.98 Theta(max)= 69.077

R(reflections)= 0.0624(23665) wR2(reflections)= 0.1675(30115)

S = 1.010 Npar= 2497

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

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	1	Report
PLAT220_ALERT_2_B	Large Non-Solvent C Ueq(max)/Ueq(min) Range	7.3	Ratio
PLAT220_ALERT_2_B	Large Non-Solvent C Ueq(max)/Ueq(min) Range	6.7	Ratio

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.64 Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.25 Report
PLAT213_ALERT_2_C	Atom O14 has ADP max/min Ratio	3.4 prolat
PLAT220_ALERT_2_C	Large Non-Solvent O Ueq(max)/Ueq(min) Range	4.4 Ratio
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	5.2 Ratio
PLAT220_ALERT_2_C	Large Non-Solvent O Ueq(max)/Ueq(min) Range	3.4 Ratio
PLAT220_ALERT_2_C	Large Non-Solvent O Ueq(max)/Ueq(min) Range	5.1 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ...	7.0 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ...	6.4 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ...	5.8 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C154 -- C162 ..	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C90 -- C114 ..	0.16 Ang.
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	0240 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C98 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C106 Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)	0252 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0097 Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H128 .. H183 ..	2.02 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N9 - H9 ..	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N11 - >H11 ..	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N12 - H12 ..	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor >N13 - >H13 ..	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N14 - H14 ..	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor N16 - H16 ..	Please Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1 Note

C80 H78 N8 O16

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: C331.8899 H325.58 Cl34.75 N
 Atom count from _chemical_formula_moiety:C331.59 H325.5899 Cl34.77 N

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum:C331.8899 H325.58 Cl34.75 N32
 Atom count from the _atom_site data: C331.8856 H323.5854 Cl34.75799

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 2
 From the CIF: _chemical_formula_sum C331.89 H325.58 Cl34.75 N32 O65
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	663.78	663.77	0.01
H	651.16	647.17	3.99

Cl	69.50	69.52	-0.02	
N	64.00	64.00	0.00	
O	130.00	130.00	0.00	
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			99 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...			56 Report
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF			Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms			18 Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 2*sigma from Zero			0.034 Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.			12.37 Why ?
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =			26 Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =			100 Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)			01 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl6	.. C224	.. 2.61 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl1A	.. C173	.. 1.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl1C	.. C170	.. 3.11 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl12	.. C173	.. 1.70 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl13	.. C154	.. 3.20 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl14	.. C173	.. 1.63 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl15	.. C173	.. 1.78 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl15	.. C26	.. 3.15 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl20	.. C165	.. 3.16 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl26	.. C173	.. 1.75 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl30	.. C173	.. 2.28 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl33	.. C145	.. 2.73 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl34	.. C173	.. 1.55 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1	.. C173	.. 2.97 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O150	.. C191	.. 2.98 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O256	.. C137	.. 2.62 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O256	.. C99	.. 2.99 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O256	.. C157	.. 3.00 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C25	.. C185	.. 3.13 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C66	.. C185	.. 3.16 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C87	.. C185	.. 2.66 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C173	.. C224	.. 1.08 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels			9 Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #			1 Check
	CL1A -CL6 -C173	1.555	1.555	1.555 44.80 Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			8 Note
	C H Cl3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			9 Note
	C H Cl3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			14 Note
	C H Cl3			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			15 Note
	C Cl			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			17 Note
	Cl			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			18 Note
	Cl			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			19 Note
	Cl			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			20 Note
	Cl			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			21 Note
	O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			23 Note
	H			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #			24 Note
	H			
PLAT791_ALERT_4_G	The Model has Chirality at C82 (Chiral SPGR)			R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C85 (Chiral SPGR)			R Verify

PLAT791_ALERT_4_G	The Model has Chirality at C86	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C90	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C98	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C102	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C103	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C107	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C123	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C129	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C130	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C153	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C167	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C176	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C101	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at C177	(Chiral SPGR)	R Verify
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		336 Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
47 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
34 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL002_ALERT_1_A The contact author's address is missing,
 _publ_contact_author_address.

PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.

PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'

PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.

PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).

PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).

PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 20/08/2014; check.def file version of 19/12/2014

Datablock I - ellipsoid plot

