

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: lgg_tdi_2cl_1th_re_0m_a_zhubin_sq

Bond precision: C-C = 0.0087 Å Wavelength=1.54178

Cell: a=15.6119(6) b=16.2521(7) c=21.8143(8)
 alpha=90 beta=104.986(3) gamma=90

Temperature: 180 K

	Calculated	Reported
Volume	5346.6(4)	5346.6(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C58 H44 Cl2 N2 O4 [+ solvent]	C58 H44 Cl2 N2 O4
Sum formula	C58 H44 Cl2 N2 O4 [+ solvent]	C58 H44 Cl2 N2 O4
Mr	903.85	903.85
Dx, g cm ⁻³	1.123	1.123
Z	4	4
Mu (mm ⁻¹)	1.443	1.443
F000	1888.0	1888.0
F000'	1895.92	
h, k, lmax	18, 19, 25	18, 19, 25
Nref	9117	8733
Tmin, Tmax	0.771, 0.917	0.571, 0.753
Tmin'	0.749	

Correction method= # Reported T Limits: Tmin=0.571 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.958 Theta(max)= 65.079

R(reflections)= 0.1180(6198)

wR2(reflections)=
0.3304(8733)

S = 1.123

Npar= 603

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

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.958 Why?



Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590

Calculated sin(theta_max)/wavelength = 0.5882

PLAT082_ALERT_2_C High R1 Value	0.12	Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.33	Report
PLAT213_ALERT_2_C Atom O008 has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C010	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C016	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C01H	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C01K	Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.4	Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00866	Ang.



Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF	Please	Check
PLAT014_ALERT_1_G No _shelx_fab_checksum Found in CIF	Please	Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	20.19	Why ?
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C009 -C00L .	1.44	Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact C100 ..C100 .	3.33	Ang.

1-x,1-y,1-z = 3_666 Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure	!	Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	108	Note

C100	O003	O004	O005	N006	N007	O008	C009
C00A	C00B	C00C	C00D	C00E	C00F	C00G	C00H
C00I	C00J	C00K	C00L	C00M	C00N	C00O	H00O
C00P	C00Q	C00R	C00S	C00T	C00U	H00U	C00V
H00V	C00W	C00X	C00Y	C00Z	H00Z	C010	C011
H011	C012	C013	H013	C014	H014	C015	H015
C016	H016	C017	C018	C019	H019	C01A	H01A
C01B	H01B	C01C	C01D	C01E	H01E	C01F	H01F
C01G	H01G	C01H	H01H	C01I	H01I	C01J	H01J
C01K	H01K	C01L	H01C	H01D	H01L	C01M	H01M
H01N	H01O	C01N	C01O	H01P	C01P	H01Q	H01R
H01S	C01Q	H01T	H01U	H01V	C01S	H01W	H01X
H01Y	C01T	H01Z	Ha	C01U	H01	Hb	Hc
C01W	H0AA	Hd	He				

PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
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PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please	Do !
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PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	3	Note
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1 1 1, -14 3 19, -4 17 9,

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

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

