

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) olsn164

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: olsn164

Bond precision:	C-C = 0.0072 A	Wavelength=0.71073
Cell:	a=19.5041(3) b=14.7989(2) c=21.4651(3)	
	alpha=90 beta=90.3628(12) gamma=90	
Temperature:	103 K	
	Calculated	Reported
Volume	6195.55(15)	6195.53(16)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C51 F51 O8 P2 Tm, C H2 Cl2	C51 F51 O8 P2 Tm, C H2 Cl2
Sum formula	C52 H2 Cl2 F51 O8 P2 Tm	C52 H2 Cl2 F51 O8 P2 Tm
Mr	2025.31	2025.31
Dx,g cm-3	2.171	2.171
Z	4	4
Mu (mm-1)	1.779	1.779
F000	3880.0	3880.0
F000'	3884.88	
h,k,lmax	27,20,29	27,20,29
Nref	17340[8675]	14562
Tmin,Tmax	0.233,0.411	0.682,1.000
Tmin'	0.162	

Correction method= # Reported T Limits: Tmin=0.682 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.84 Theta(max)= 29.574

R(reflections)= 0.0285(14207) wR2(reflections)= 0.0754(14562)

S = 1.045 Npar= 1073

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

PLAT213_ALERT_2_B	Atom F8	has ADP max/min Ratio	4.4	prolat
PLAT434_ALERT_2_B	Short Inter HL..HL Contact F7	.. F51B ..	2.44	Ang.
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Th(Min)	...	11	Report
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	6	Check

Alert level C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	8.07	Note
PLAT213_ALERT_2_C	Atom F7	has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom F9	has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom F46	has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom F47	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom F48	has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom F50B	has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom F51A	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C10	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C11	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent F	Ueq(max)/Ueq(min) Range	5.4	Ratio
PLAT915_ALERT_3_C	Low Friedel Pair Coverage	68	%
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much smaller I(calc)	.	1	Check
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.88A From Tml	1.54	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.97A From O2	-0.47	eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...	7	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	1.00	mm
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT242_ALERT_2_G	Low	Ueq as Compared to Neighbors for	C41	Check
PLAT242_ALERT_2_G	Low	Ueq as Compared to Neighbors for	C42	Check
PLAT242_ALERT_2_G	Low	Ueq as Compared to Neighbors for	C46	Check
PLAT242_ALERT_2_G	Low	Ueq as Compared to Neighbors for	C47	Check
PLAT242_ALERT_2_G	Low	Ueq as Compared to Neighbors for	C51	Check
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	3	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F18 .. C11 ..	2.90	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F33 .. C27 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F34 .. C36 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F44 .. C3 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F44 .. C2 ..	2.94	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F4 .. F22 ..	2.78	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F7 .. F42 ..	2.79	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F8 .. F23 ..	2.69	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F8 .. F39 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F17 .. F50B ..	2.77	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F22 .. F33 ..	2.81	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F24 .. F37 ..	2.76	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F29 .. F50A ..	2.81	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F29 .. F51B ..	2.82	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F29 .. F32 ..	2.83	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F30 .. F34 ..	2.78	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F32 .. F50B ..	2.77	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F38 .. F50A ..	2.65	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	86	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

4 **ALERT level B** = A potentially serious problem, consider carefully

16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

29 **ALERT level G** = General information/check it is not something unexpected

0 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
7 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*, 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.

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