

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) olsn165

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: olsn165

Bond precision:	C-C = 0.0115 A	Wavelength=0.71073
Cell:	a=19.5641(4)	b=14.7311(4) c=21.5669(6)
	alpha=90	beta=90.046(2) gamma=90
Temperature:	184 K	
	Calculated	Reported
Volume	6215.6(3)	6215.6(3)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C51 F51 O8 P2 Sm, C H2 Cl2	C51 F51 O8 P2 Sm, C H2 Cl2
Sum formula	C52 H2 Cl2 F51 O8 P2 Sm	C52 H2 Cl2 F51 O8 P2 Sm
Mr	2006.74	2006.73
Dx,g cm-3	2.145	2.144
Z	4	4
Mu (mm-1)	1.291	1.291
F000	3852.0	3852.0
F000'	3857.48	
h,k,lmax	24,18,26	24,18,26
Nref	12713[6361]	8632
Tmin,Tmax	0.465,0.597	0.385,1.000
Tmin'	0.352	

Correction method= # Reported T Limits: Tmin=0.385 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.36/0.68 Theta(max)= 26.367

R(reflections)= 0.0356(8380) wR2(reflections)= 0.1059(8632)

S = 1.035 Npar= 1045

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

PLAT090_ALERT_3_B	Poor Data / Parameter Ratio (Zmax > 18)	5.98	Note
PLAT915_ALERT_3_B	Low Friedel Pair Coverage	38	%
PLAT919_ALERT_3_B	Reflection # Likely Affected by the Beamstop ...	1	Check
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	2	Check

Alert level C

PLAT213_ALERT_2_C	Atom F47	has ADP max/min Ratio	3.7	prolat
PLAT220_ALERT_2_C	Large Non-Solvent F	Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C47	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C52	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0115	Ang.	
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Th(Min) ...	10	Report	
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	77	Report	
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much smaller I(calc) .	2	Check	
PLAT972_ALERT_2_C	Check Calcd Residual Density 1.13A From Sml	-1.77	eA-3	
PLAT972_ALERT_2_C	Check Calcd Residual Density 0.94A From Sml	-1.63	eA-3	

Alert level G

PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.80	mm	
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	C51	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F34 .. C18 ..	2.94	Ang.	
PLAT432_ALERT_2_G	Short Inter X...Y Contact F43 .. C20 ..	2.91	Ang.	
PLAT432_ALERT_2_G	Short Inter X...Y Contact F43 .. C21 ..	2.95	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F19 ..	2.76	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F51 ..	2.83	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 .. F32 ..	2.84	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F9 .. F36 ..	2.81	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F13 .. F25 ..	2.78	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F14 .. F33 ..	2.80	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F15 .. F34 ..	2.78	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F15 .. F33 ..	2.84	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F17 .. F41 ..	2.83	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F27 .. F42 ..	2.80	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F28 .. F40 ..	2.82	Ang.	
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F38 .. F45 ..	2.74	Ang.	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	24	Note	

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 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.

