

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P22313\_t5

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: P22313\_t5**

Bond precision:	C-C = 0.0099 A		Wavelength=1.54178
Cell:	a=29.4547 (10)	b=6.6980 (3)	c=8.0253 (3)
	alpha=90	beta=95.5699 (18)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	1575.82 (11)	1575.82 (11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C38 H14 F10 O4 S2	?
Sum formula	C38 H14 F10 O4 S2	C38 H14 F10 O4 S2
Mr	788.61	788.61
Dx, g cm <sup>-3</sup>	1.662	1.662
Z	2	2
Mu (mm <sup>-1</sup> )	2.483	2.483
F000	792.0	792.0
F000'	796.49	
h, k, l <sub>max</sub>	37, 8, 10	37, 8, 9
Nref	3350	4344
Tmin, Tmax	0.789, 0.862	0.262, 0.427
Tmin'	0.716	

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Correction method= # Reported T Limits: Tmin=0.262 Tmax=0.427
AbsCorr = MULTI-SCAN
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Data completeness= 1.297                      Theta (max)= 77.366

R(reflections)= 0.1385( 3811)	wR2(reflections)= 0.3927( 4344)
S = 3.109	Npar= 264

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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.

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### Alert level B

PLAT084\_ALERT\_3\_B High wR2 Value (i.e. > 0.25) ..... 0.39 Report

**Author Response: The crystal quality was exceptionally low and the data quality reflects this.**

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 2.37 eA-3

**Author Response: The crystal quality was exceptionally low and not all twinning could be resolved (there likely is a third twin domain). The highest residual electron density peaks are not in sensible positions where they could correspond to additional atoms or missed disorder. More likely, those maxima are artefacts of unresolved non-merohedral twinning.**

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### Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00

Goodness of fit given = 3.109

PLAT029\_ALERT\_3\_C \_diffn\_measured\_fraction\_theta\_full value Low . 0.972 Why?  
PLAT082\_ALERT\_2\_C High R1 Value ..... 0.14 Report  
PLAT085\_ALERT\_2\_C SHELXL Default Weighting Scheme is not Optimized Please Check  
PLAT087\_ALERT\_2\_C Unsatisfactory S value (Too High) ..... 3.11 Check  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.58 Report  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00994 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 8.177 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.611 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 80 Report

0	4	0,	0	8	0,	1	8	0,	2	8	0,	-5	0	2,	-4	0	2,
-2	6	3,	2	7	3,	9	6	3,	-11	0	4,	-9	1	4,	-6	0	4,
-5	0	4,	-3	0	4,	-3	7	4,	-2	7	4,	0	6	4,	0	7	4,
1	6	4,	1	7	4,	2	6	4,	2	7	4,	3	6	4,	3	7	4,
4	6	4,	5	6	4,	6	7	4,	-6	6	5,	-1	6	5,	0	6	5,
1	6	5,	2	6	5,	3	6	5,	4	6	5,	-9	6	6,	-8	5	6,
-8	6	6,	-7	5	6,	-7	6	6,	-5	0	6,	-4	0	6,	-4	5	6,
-4	6	6,	-3	0	6,	-3	6	6,	-2	6	6,	-1	6	6,	0	6	6,
1	6	6,	2	6	6,	4	6	6,	-3	3	7,	-1	5	7,	-8	3	8,
-7	3	8,	-6	2	8,	-6	3	8,	-5	3	8,	-4	2	8,	-3	2	8,
-1	3	8,	0	2	8,	0	3	8,	1	2	8,	1	3	8,	2	3	8,
5	4	8,	6	3	8,	7	3	8,	13	0	8,	-9	2	9,	-7	2	9,
-6	2	9,	-5	2	9,	-2	2	9,	0	2	9,	1	2	9,	2	2	9,
3	2	9,	5	2	9,												

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### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	29	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	5	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT301_ALERT_3_G	Main Residue Disorder ..... (Resd 1)	7%	Note
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C5 - C6 .	1.44	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact S1A ..C4 .	3.26	Ang.
	$x, 3/2-y, 1/2+z =$	4_576	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 ..F4 .	2.79	Ang.
	$2-x, -1/2+y, 3/2-z =$	2_746	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	426	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	91	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.4	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	7.966	Note
	Predicted wR2: Based on SigI**2 4.92 or SHELX Weight 12.63		

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 2 **ALERT level B** = A potentially serious problem, consider carefully  
 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 18 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 11 ALERT type 3 Indicator that the structure quality may be low  
 6 ALERT type 4 Improvement, methodology, query or suggestion  
 1 ALERT type 5 Informative message, check
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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.

