

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_285

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: exp\_285

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Bond precision:      C-C = 0.0033 A

Wavelength=0.71073

Cell:                      a=9.8852 (3)                      b=10.0996 (4)                      c=16.0526 (4)  
                              alpha=99.813 (3)                      beta=94.164 (2)                      gamma=102.911 (3)  
Temperature:              100 K

|                | Calculated                           | Reported                            |
|----------------|--------------------------------------|-------------------------------------|
| Volume         | 1529.01 (9)                          | 1529.01 (9)                         |
| Space group    | P -1                                 | P -1                                |
| Hall group     | -P 1                                 | -P 1                                |
| Moiety formula | C28 H19 F3 Fe O4 P, B F4 [+ solvent] | C28 H19 F3 Fe O4 P, B F4, 1[CH2CL2] |
| Sum formula    | C28 H19 B F7 Fe O4 P [+ solvent]     | C29 H21 B Cl2 F7 Fe O4 P            |
| Mr             | 650.06                               | 734.99                              |
| Dx, g cm-3     | 1.412                                | 1.596                               |
| Z              | 2                                    | 2                                   |
| Mu (mm-1)      | 0.619                                | 0.798                               |
| F000           | 656.0                                | 740.0                               |
| F000'          | 657.33                               |                                     |
| h, k, lmax     | 11, 12, 19                           | 11, 12, 19                          |
| Nref           | 5678                                 | 5636                                |
| Tmin, Tmax     | 0.702, 0.894                         | 0.981, 0.996                        |
| Tmin'          | 0.613                                |                                     |

Correction method= # Reported T Limits: Tmin=0.981 Tmax=0.996  
AbsCorr = GAUSSIAN

Data completeness= 0.993

Theta (max)= 25.500

R(reflections)= 0.0378( 4647)

wR2(reflections)=  
0.1044( 5636)

S = 1.072

Npar= 379

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 C

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of B1 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 37 Report

|      |     |      |    |      |    |      |    |      |    |      |    |
|------|-----|------|----|------|----|------|----|------|----|------|----|
| 7-11 | 3,  | 7-10 | 3, | 6-11 | 4, | 7-11 | 4, | 6-10 | 4, | 7-10 | 4, |
| 8-10 | 4,  | 6 -9 | 4, | 6-11 | 5, | 6-10 | 5, | 7-10 | 5, | 8-10 | 5, |
| 6 -9 | 5,  | 7 -9 | 5, | 5-11 | 6, | 6-11 | 6, | 5-10 | 6, | 6-10 | 6, |
| 7-10 | 6,  | 8-10 | 6, | 5 -9 | 6, | 6 -9 | 6, | 7 -9 | 6, | 5-11 | 7, |
| 6-11 | 7,  | 5-10 | 7, | 6-10 | 7, | 7-10 | 7, | 6 -9 | 7, | 7 -9 | 7, |
| 5-11 | 8,  | 6-10 | 8, | 7-10 | 8, | 5-11 | 9, | 6-10 | 9, | 7-10 | 9, |
| 6-10 | 10, |      |    |      |    |      |    |      |    |      |    |



### Alert level G

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: C29 H21 B1 Cl2 F7 Fe1 O4 P1

Atom count from the \_atom\_site data: C28 H19 B1 F7 Fe1 O4 P1

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 2

From the CIF: \_chemical\_formula\_sum C29 H21 B Cl2 F7 Fe O4 P

TEST: Compare cell contents of formula and atom\_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|------|
| C    | 58.00     | 56.00     | 2.00 |
| H    | 42.00     | 38.00     | 4.00 |
| B    | 2.00      | 2.00      | 0.00 |
| Cl   | 4.00      | 0.00      | 4.00 |
| F    | 14.00     | 14.00     | 0.00 |
| Fe   | 2.00      | 2.00      | 0.00 |
| O    | 8.00      | 8.00      | 0.00 |
| P    | 2.00      | 2.00      | 0.00 |

PLAT041\_ALERT\_1\_G Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C28 H19 B F7 Fe O4 P

Rep.: C29 H21 B Cl2 F7 Fe O4 P

PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: C28 H19 F3 Fe O4 P, B F4

Rep.: C28 H19 F3 Fe O4 P, B F4, 1[CH2CL2]

PLAT051\_ALERT\_1\_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 22.45 %

PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report

PLAT190\_ALERT\_3\_G A Non-default RIGU Restraint Value for First Par 0.0020 Report

PLAT190\_ALERT\_3\_G A Non-default RIGU Restraint Value for SecondPar 0.0020 Report

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fel --C8 . 7.3 s.u.

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fel --C9 . 7.6 s.u.

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fel --C10 . 7.9 s.u.

|                                                                    |             |
|--------------------------------------------------------------------|-------------|
| PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure | 226 A**3    |
| PLAT793_ALERT_4_G Model has Chirality at C6 (Centro SpGr)          | S Verify    |
| PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II)              | 1.97 Info   |
| PLAT860_ALERT_3_G Number of Least-Squares Restraints .....         | 309 Note    |
| PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed | ! Info      |
| PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). | 2 Note      |
| 0 1 0, 0 0 1,                                                      |             |
| PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600  | 3 Note      |
| PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File | 1 Note      |
| 0 1 0,                                                             |             |
| PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. | 51.0 Degree |
| PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....       | 1.845 Note  |
| Predicted wR2: Based on SigI**2 5.66 or SHELX Weight               | 9.74        |
| PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. | 10 Info     |

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

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

Datablock exp\_285 - ellipsoid plot

