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: ld15

```
Bond precision:  C-C = 0.0106 A          Wavelength=0.71073

Cell:            a=20.6177(3)     b=20.6177(3)     c=11.7467(3)
                 alpha=90         beta=90          gamma=90
Temperature:     123 K
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	Calculated	Reported
Volume	4993.40(19)	4993.40(16)
Space group	P -4 n 2	P-4n2
Hall group	P -4 -2n	?
Moiety formula	C16 H16 Cs Fe N8 O8 S2	?
Sum formula	C16 H16 Cs Fe N8 O8 S2	C16 H16 Cs Fe N8 O8 S2
Mr	701.25	701.25
Dx,g cm-3	1.866	1.866
Z	8	8
Mu (mm-1)	2.266	2.266
F000	2760.0	2760.0
F000’	2762.77	
h,k,lmax	32,32,18	32,32,18
Nref	10093[5418]	10084
Tmin,Tmax	0.672,0.762	0.660,0.773
Tmin’	0.629	

```
Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.773
AbsCorr = MULTI-SCAN

Data completeness= 1.86/1.00      Theta(max)= 33.870

R(reflections)= 0.0747( 8551)     wR2(reflections)= 0.2314( 10084)

S = 1.064                 Npar= 331
```

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

PLAT420_ALERT_2_B D-H Without Acceptor O7 -- H7A ... Please Check

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -4.962
Test value = -4.125
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -4.96 eA-3
PLAT213_ALERT_2_C Atom O8 has ADP max/min Ratio ..... 3.6 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 Cs Ueq(max)/Ueq(min) Range 5.2 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 5.8 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cs1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01057 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X H9A .. H15 .. 2.10 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 77 Ang3
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C16 H16 Cs Fe N8 O8 S2

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 10 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 33.24 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 3 Units
PLAT300_ALERT_4_G Atom Site Occupancy of *Cs2 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H8A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H8B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H9A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H9B is Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 1 Note
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C16 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O4 .. C15 .. 2.91 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.52 Ratio
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: FE1 -- CS1 .. 4.30 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: S2 -- CS2 .. 4.07 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: CS2 -- S2 .. 4.07 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: CS2 -- CS2 .. 4.37 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: CS2 -- CS2 .. 4.37 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: CS2 -- CS2 .. 5.55 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (III) ..... 4.42 Note
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 104 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 12 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 15 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
  8 ALERT type 4 Improvement, methodology, query or suggestion
  4 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.

PLATON version of 30/03/2016; check.def file version of 30/03/2016

Datablock ld15 - ellipsoid plot