

No syntax errors found.
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Datablock: c4ssf4_work2

Bond precision: C-C = 0.0062 Å Wavelength=0.71073
Cell: a=19.5646(5) b=22.6693(5) c=25.1428(6)
alpha=90 beta=116.6093(9) gamma=90
Temperature: 140 K

	Calculated	Reported
Volume	9970.1(4)	9970.1(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C84 H148 Fe4 O18 S4	C84 H148 Fe4 O18 S4
Sum formula	C84 H148 Fe4 O18 S4	C84 H148 Fe4 O18 S4
Mr	1797.72	1797.66
Dx, g cm ⁻³	1.198	1.198
Z	4	4
Mu (mm ⁻¹)	0.711	0.711
F000	3856.1	3856.0
F000'	3865.06	
h, k, lmax	24, 27, 31	24, 27, 31
Nref	9834	9810
Tmin, Tmax	0.676, 0.892	0.717, 0.895
Tmin'	0.660	

Correction method= # Reported T Limits: Tmin=0.717
Tmax=0.895 AbsCorr = MULTI-SCAN
Data completeness= 0.998 Theta(max)= 26.024
R(reflections)= 0.0565(7858) wR2(reflections)= 0.1855(9810)
S = 1.058 Npar= 555

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

[PLAT213_ALERT_2_C](#) Atom C17 has ADP max/min Ratio 3.3 prolat
[PLAT220_ALERT_2_C](#) NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.1 Ratio
[PLAT222_ALERT_3_C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C4 Check

And 4 other PLAT242 Alerts

[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C14 Check
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C22 Check
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C30 Check

[PLAT341_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.00624 Ang.
[PLAT910_ALERT_3_C](#) Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
[PLAT918_ALERT_3_C](#) Reflection(s) with I(obs) much Smaller I(calc) 3 Check
[PLAT922_ALERT_1_C](#) wR2 in the CIF and FCF Differ by 0.0013 Check
[PLAT934_ALERT_3_C](#) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
[PLAT977_ALERT_2_C](#) Check Negative Difference Density on H39E -0.32 eA-3

Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 30 Note
[PLAT003_ALERT_2_G](#) Number of Uiso or Uij Restrained non-H Atoms ... 24 Report
[PLAT068_ALERT_1_G](#) Reported F000 Differs from Calcd (or Missing)... Please Check
[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 20.00 Why ?
[PLAT158_ALERT_4_G](#) The Input Unitcell is NOT Standard/Reduced Please Check
[PLAT168_ALERT_4_G](#) The CIF-Embedded .res File Contains EXYZ Records 1 Report
[PLAT172_ALERT_4_G](#) The CIF-Embedded .res File Contains DFIX Records 1 Report
[PLAT175_ALERT_4_G](#) The CIF-Embedded .res File Contains SAME Records 3 Report
[PLAT176_ALERT_4_G](#) The CIF-Embedded .res File Contains SADI Records 2 Report
[PLAT187_ALERT_4_G](#) The CIF-Embedded .res File Contains RIGU Records 1 Report
[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for S1A --S2A . 12.8 s.u.
[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for S2A --C39A . 6.8 s.u.
[PLAT301_ALERT_3_G](#) Main Residue Disorder(Resd 1) 20% Note
[PLAT410_ALERT_2_G](#) Short Intra H...H Contact H3A ..H38F . 2.10 Ang.
[PLAT412_ALERT_2_G](#) Short Intra XH3 .. XHn H9 ..H29C . 2.09 Ang.
[PLAT413_ALERT_2_G](#) Short Inter XH3 .. XHn H15A ..H39D . 1.98 Ang.
1/2-x, 1/2+y, 1/2-z = 4_555 Check

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PLAT413 ALERT 2 G Short Inter XH3 .. XHn      H33B      ..H41F      .      1.70 Ang.
                                           -x,-y,-z =      5_555 Check
PLAT432 ALERT 2 G Short Inter X...Y Contact    S2B      ..C35      .      3.12 Ang.
                                           x,-y,1/2+z =      6_556 Check
PLAT432 ALERT 2 G Short Inter X...Y Contact    C33      ..C41C      .      3.17 Ang.
                                           -x,-y,-z =      5_555 Check
PLAT774 ALERT 1 G Check X-Y Bond in CIF: Fe2      --Fe3      ..      5.32 Ang.
PLAT774 ALERT 1 G Check X-Y Bond in CIF: Fe3      --Fe3      ..      5.32 Ang.
PLAT789 ALERT 4 G Atoms with Negative atom_site_disorder_group #      54 Check
PLAT794 ALERT 5 G Tentative Bond Valency for Fe1      (III)      .      3.28 Info
And 2 other PLAT794 Alerts

PLAT794 ALERT 5 G Tentative Bond Valency for Fe2      (III)      .      3.19 Info
PLAT794 ALERT 5 G Tentative Bond Valency for Fe3      (III)      .      3.21 Info

PLAT802 ALERT 4 G CIF Input Record(s) with more than 80 Characters      1 Info
PLAT860 ALERT 3 G Number of Least-Squares Restraints .....      86 Note
PLAT912 ALERT 4 G Missing # of FCF Reflections Above STh/L= 0.600      17 Note
PLAT965 ALERT 2 G The SHELXL WEIGHT Optimisation has not Converged      Please Check
PLAT978 ALERT 2 G Number C-C Bonds with Positive Residual Density.      1 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
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
30 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 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
9 ALERT type 4 Improvement, methodology, query or suggestion
3 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

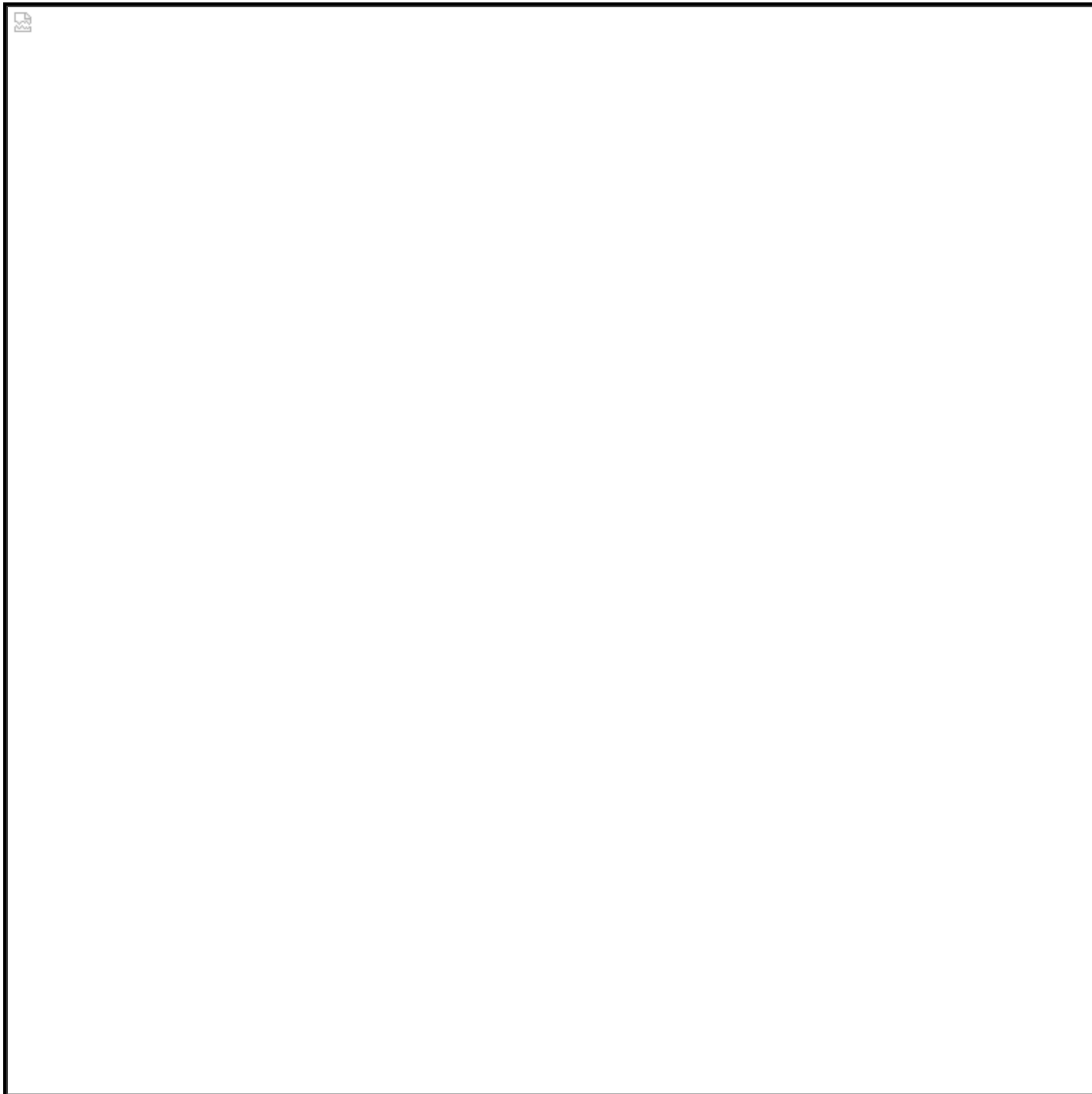
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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 18/09/2020; check.def file version of 20/08/2020

Datablock c4ssf4_work2 - ellipsoid plot



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