

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: Fe4SCN_2_work4

Bond precision: C-C = 0.0037 Å Wavelength=0.71073
Cell: a=27.8089(12) b=17.3432(8) c=20.7771(8)
alpha=90 beta=117.3181(14) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	8903.1(7)	8903.1(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C78 H130 Fe4 N2 O18 S2	C78 H130 Fe4 N2 O18 S2
Sum formula	C78 H130 Fe4 N2 O18 S2	C78 H130 Fe4 N2 O18 S2
Mr	1671.36	1671.35
Dx, g cm ⁻³	1.247	1.247
Z	4	4
Mu (mm ⁻¹)	0.747	0.747
F000	3568.0	3568.0
F000'	3575.90	
h, k, lmax	36, 22, 27	36, 22, 27
Nref	10803	10747
Tmin, Tmax	0.675, 0.770	0.603, 0.780
Tmin'	0.632	

Correction method= # Reported T Limits: Tmin=0.603
Tmax=0.780 AbsCorr = MULTI-SCAN
Data completeness= 0.995 Theta(max)= 28.043
R(reflections)= 0.0438 (8194) wR2(reflections)= 0.1352 (10747)
S = 1.069 Npar= 501

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

[PLAT910_ALERT_3_B](#) Missing # of FCF Reflection(s) Below Theta(Min). 19 Note

Author Response: Low-order reflections (partly) obscured by the beam stopper and rejected as outliers by SADABS or deliberately omitted from the final least-squares refinement based on Iobs << Icalc.

Alert level C

[PLAT094_ALERT_2_C](#) Ratio of Maximum / Minimum Residual Density 2.22 Report
[PLAT220_ALERT_2_C](#) NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio
[PLAT222_ALERT_3_C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C26 Check
[PLAT242_ALERT_2_C](#) Low 'MainMol' Ueq as Compared to Neighbors of C30 Check
[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report
[PLAT922_ALERT_1_C](#) wR2 in the CIF and FCF Differ by 0.0012 Check

Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 8 Note
[PLAT003_ALERT_2_G](#) Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 6.38 Why ?
[PLAT128_ALERT_4_G](#) Alternate Setting for Input Space Group C2/c 12/a Note
[PLAT171_ALERT_4_G](#) The CIF-Embedded .res File Contains EADP Records 1 Report
[PLAT175_ALERT_4_G](#) The CIF-Embedded .res File Contains SAME Records 1 Report
[PLAT187_ALERT_4_G](#) The CIF-Embedded .res File Contains RIGU Records 2 Report
[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for S1 --C39 . 7.3 s.u.
[PLAT301_ALERT_3_G](#) Main Residue Disorder(Resd 1) 8% Note
[PLAT412_ALERT_2_G](#) Short Intra XH3 .. XHn H6 ..H15C . 2.11 Ang.
x, y, z = 1_555 Check
[PLAT774_ALERT_1_G](#) Check X-Y Bond in CIF: Fe2 --Fe3 .. 5.43 Ang.
[PLAT774_ALERT_1_G](#) Check X-Y Bond in CIF: Fe3 --Fe3 .. 5.22 Ang.
[PLAT794_ALERT_5_G](#) Tentative Bond Valency for Fe1 (III) . 3.24 Info

And 2 other PLAT794 Alerts

[PLAT794_ALERT_5_G](#) Tentative Bond Valency for Fe2 (III) . 3.23 Info
[PLAT794_ALERT_5_G](#) Tentative Bond Valency for Fe3 (III) . 3.18 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 42 Note

PLAT912	ALERT	4	G	Missing # of FCF Reflections Above STh/L= 0.600	29	Note
PLAT913	ALERT	3	G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933	ALERT	2	G	Number of OMIT Records in Embedded .res File ...	14	Note
PLAT941	ALERT	3	G	Average HKL Measurement Multiplicity	4.4	Low
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.	3	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 7 **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

3 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
 7 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

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

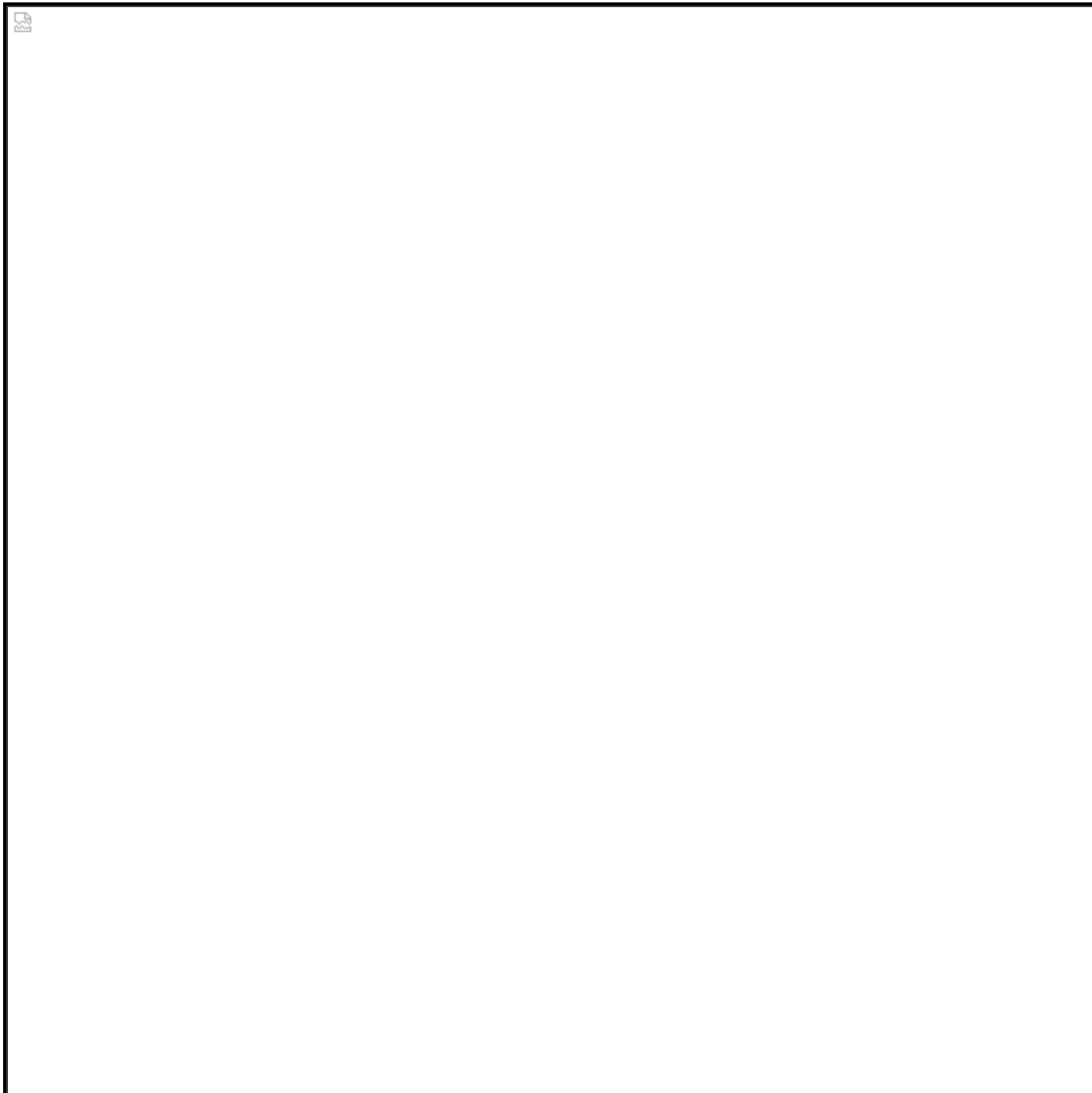
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 Fe4SCN_2_work4 - ellipsoid plot



[Download CIF editor \(publCIF\) from the IUCr](#)
[Download CIF editor \(enCIFer\) from the CCDC](#)
[Test a new CIF entry](#)