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: mo_d8v3475_2_0mtotal_a

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Bond precision:  C-C = 0.0124 A          Wavelength=0.71073

Cell:              a=12.274(3)      b=16.101(3)      c=20.668(4)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
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	Calculated	Reported
Volume	4084.5(15)	4084.4(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C30 H24 F18 Fe O12 Pr	0.5(C30 H24 F18 Fe O12 Pr)
Sum formula	C30 H24 F18 Fe O12 Pr	C15 H12 F9 Fe0.50 O6 Pr0.50
Mr	1115.25	557.63
Dx,g cm-3	1.814	1.814
Z	4	8
Mu (mm-1)	1.671	1.671
F000	2188.0	2188.0
F000’	2190.42	
h,k,lmax	15,19,25	15,19,25
Nref	7801[4344]	7782
Tmin,Tmax	0.420,0.529	0.250,0.746
Tmin’	0.318	

```
Correction method= # Reported T Limits: Tmin=0.250 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00      Theta(max)= 25.741

R(reflections)= 0.0369( 7235)     wR2(reflections)= 0.0956( 7782)

S = 1.059                 Npar= 566
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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.

Alert level C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.67	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.17	Report
PLAT213_ALERT_2_C	Atom F019 has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom F12 has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom F14 has ADP max/min Ratio	3.7	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for F15 --C01P .	5.2	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F13 --C01P	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F17 --C01M	0.19	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01237	Ang.

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please	Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.66	mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.51	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C00N	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C01A	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C01C	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C01M	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C01P	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C014	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	66	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Pr01 (III) .	3.56	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe02 (III) .	3.17	Info
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and s.u.	0.02	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12	Note

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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
10	**ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20	**ALERT level G** = General information/check it is not something unexpected

5	ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14	ALERT type 2 Indicator that the structure model may be wrong or deficient
3	ALERT type 3 Indicator that the structure quality may be low
6	ALERT type 4 Improvement, methodology, query or suggestion
2	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 23/04/2018; check.def file version of 23/04/2018

Datablock mo_d8v3475_2_0mtotal_a - ellipsoid plot