checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGRB4

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: SGGRB4

Bond precision: C-C = 0.0113 A   Wavelength=0.71073

Cell: a=11.6885(13)   b=16.2795(16)   c=15.0773(17)
                 alpha=90   beta=110.538(4)   gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	2686.6(5)	2686.6(5)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H38 B4 Fe O3 W2	C23 H38 B4 Fe O3 W2
Sum formula	C23 H38 B4 Fe O3 W2	C23 H38 B4 Fe O3 W2
Mr	829.30	829.32
Dx,g cm-3	2.050	2.050
Z	4	4
Mu (mm-1)	9.097	9.097
F000	1576.0	1576.0
F000'	1571.60	
h,k,lmax	15,21,19	15,21,19
Nref	6155	6147
Tmin,Tmax	0.047,0.761	0.388,0.761
Tmin'	0.004	

Correction method= # Reported T Limits: Tmin=0.388 Tmax=0.761
AbsCorr = MULTI-SCAN

Data completeness= 0.999   Theta(max)= 27.484

R(reflections)= 0.0379(5606)   wR2(reflections)= 0.1236(6147)

S = 1.063   Npar= 320

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

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PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01125 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          8 Note
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.05A    From B43          2.33 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.26A    From W1           2.17 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.17A    From W1           2.14 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.40A    From W2           1.99 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00A    From B44          1.92 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.33A    From W2           1.77 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.28A    From W2           1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.98A    From B44          1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18A    From W2           1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.57A    From B44          1.59 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.19A    From W2           1.58 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.71A    From W2           1.57 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.81A    From W2          -2.13 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.84A    From W1          -2.10 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.00A    From W1          -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From W2          -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.62A    From W2          -2.00 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.57A    From W1          -1.98 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.54A    From W2          -1.87 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.00A    From W1          -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.09A    From W2          -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.18A    From B41         -1.72 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82A    From B43         -1.68 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.66A    From W2          -1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.96A    From C11         -1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.16A    From W1          -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.08A    From W2          -1.57 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From C2          -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.72A    From W1          -1.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10A           -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16C           -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19A           -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H20B           -0.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H41            -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H42            -0.49 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.        0 Info
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    10.04 Why ?
PLAT303_ALERT_2_G Full Occupancy Atom H41B      with # Connections     2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H41C      with # Connections     2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H42B      with # Connections     2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H42C      with # Connections     2.00 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C20 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.11 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      308 Check
           W2   -B41  -H41B    1.555   1.555   1.555         35.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      313 Check
           W1   -B41  -H41C    1.555   1.555   1.555         33.00 Deg.
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        1 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
  39 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected
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 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
42 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
 4 ALERT type 4 Improvement, methodology, query or suggestion
 0 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 06/01/2019; check.def file version of 19/12/2018