checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hijazi3m

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: hijazi3m

Bond precision:  C-C = 0.0185 A        Wavelength=0.71073

Cell:              a=20.930(3)     b=14.8360(19)     c=15.807(2)
                    alpha=90       beta=101.705(2)    gamma=90
Temperature:     295 K

                    Calculated     Reported
Volume               4806.3(11)     4806.3(11)
Space group               P 21/c     P2(1)/c
Hall group                -P 2yc      -P 2yc
Moietry formula         C53 H38 Co F2 N2 O5 S2     C53 H38 Co F2 N2 O5 S2
Sum formula              C53 H38 Co F2 N2 O5 S2     C53 H38 Co F2 N2 O5 S2
Mr                     943.90       943.90
Dx,g cm-3             1.304         1.304
Z                      4             4
Mu (mm-1)                0.500       0.500
F000                    1948.0      1948.0
F000’                   1951.22     
\(h,k,l\)max           26,18,20      26,18,20
Nref                   10501        10468
Tmin,Tmax              0.767,0.975  0.777,0.975
Tmin’                  0.767        

Correction method= # Reported T Limits: Tmin=0.777 Tmax=0.975
AbsCorr = MULTI-SCAN

Data completeness= 0.997       Theta(max)= 27.000
R(reflections)= 0.1941( 7302)   wR2(reflections)= 0.4718( 10468)
\(S = 1.575 \quad Npar= 603\)

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 A**

- **RFACR01_ALERT_3_A** The value of the weighted R factor is > 0.45
  - Weighted R factor given 0.472

- **PLAT084_ALERT_3_A** High wR2 Value (i.e. > 0.25) 0.47 Report

- **PLAT215_ALERT_4_A** Disordered C40 has ADP max/min Ratio 5.4 Note

- **PLAT234_ALERT_4_A**
  - Large Hirshfeld Difference S2 -- O6 0.40 Ang.
  - Large Hirshfeld Difference S2 -- C40 0.44 Ang.
  - Large Hirshfeld Difference C46 -- C47 0.33 Ang.

- **PLAT241_ALERT_2_A** High ‘MainMol’ Ueq as Compared to Neighbors of S1 Check

- **PLAT902_ALERT_1_A** No (Interpretable) Reflections found in FCF Please Check

**Alert level B**

- **RFACG01_ALERT_3_B** The value of the R factor is > 0.15
  - R factor given 0.194

- **PLAT082_ALERT_2_B** High R1 Value 0.19 Report

- **PLAT213_ALERT_4_B**
  - Atom C47 has ADP max/min Ratio 4.7 prolat

- **PLAT234_ALERT_4_B**
  - Large Hirshfeld Difference C37 -- C38 0.28 Ang.

- **PLAT241_ALERT_2_B**
  - High ‘MainMol’ Ueq as Compared to Neighbors of S2 Check
  - High ‘MainMol’ Ueq as Compared to Neighbors of O5 Check

- **PLAT242_ALERT_2_B**
  - Low ‘MainMol’ Ueq as Compared to Neighbors of C17 Check
  - Low ‘MainMol’ Ueq as Compared to Neighbors of C37 Check

- **PLAT241_ALERT_2_B**
  - High ‘MainMol’ Ueq as Compared to Neighbors of O1 Check

**Alert level C**

- **DIFMX01_ALERT_2_C** The maximum difference density is > 0.1*ZMAX*0.75
  - _refine_diff_density_max given = 2.149
  - Test value = 2.025

- **DIFMX02_ALERT_1_C** The maximum difference density is > 0.1*ZMAX*0.75
  - The relevant atom site should be identified.

- **SHFSU01_ALERT_2_C**
  - The absolute value of parameter shift to su ratio > 0.05
  - Absolute value of the parameter shift to su ratio given 0.078
  - Additional refinement cycles may be required.

- **PLAT080_ALERT_2_C** Maximum Shift/Error 0.08 Why ?

- **PLAT094_ALERT_2_C** Ratio of Maximum / Minimum Residual Density 3.14 Report

- **PLAT213_ALERT_4_C**
  - Atom S1 has ADP max/min Ratio 3.0 eÅ-3
  - Atom C44 has ADP max/min Ratio 3.4 eÅ-3

- **PLAT220_ALERT_2_C**
  - Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio

- **PLAT230_ALERT_2_C**
  - Hirshfeld Test Diff for C45 -- C46 7.0 s.u.

- **PLAT234_ALERT_4_C**
  - Large Hirshfeld Difference S1 -- C17 0.21 Ang.
  - Large Hirshfeld Difference F2 -- C26 0.25 Ang.
  - Large Hirshfeld Difference O5 -- C21 0.22 Ang.
  - Large Hirshfeld Difference N1 -- C41 0.17 Ang.
  - Large Hirshfeld Difference N2 -- C52 0.18 Ang.
  - Large Hirshfeld Difference C7 -- C8 0.16 Ang.
  - Large Hirshfeld Difference C22 -- C23 0.18 Ang.
  - Large Hirshfeld Difference C23 -- C31 0.18 Ang.
  - Large Hirshfeld Difference C24 -- C25 0.23 Ang.
  - Large Hirshfeld Difference C25 -- C26 0.25 Ang.
  - Large Hirshfeld Difference C26 -- C29 0.16 Ang.
  - Large Hirshfeld Difference C30 -- C33 0.18 Ang.
  - Large Hirshfeld Difference C34 -- C39 0.18 Ang.
  - Large Hirshfeld Difference C36 -- C37 0.24 Ang.
  - Large Hirshfeld Difference C38 -- C39 0.22 Ang.
  - Large Hirshfeld Difference C43 -- C44 0.20 Ang.
  - Large Hirshfeld Difference C44 -- C45 0.18 Ang.
  - Large Hirshfeld Difference C51 -- C52 0.23 Ang.

- **PLAT241_ALERT_2_C**
  - High ‘MainMol’ Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O4 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C44 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C46 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C47 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C50 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C51 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
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 C34 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C42 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C45 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C48 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C52 Check
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C52 - C54 .. 1.41 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C47 - C48 .. 1.56 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 46 Ang3

Alert level G
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do!
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_1_G SHEXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for S1 -- O3 .. 14.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Col -- O5 .. 5.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of *O3 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O6 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C20 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C40 is Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ............ Percentage = 3 Note
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C41 -C49 1.44 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C24 -C29 0.18 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C41 -C49 0.32 Ang.
PLAT899_ALERT_4_G SHEXL97 is Deprecated and Succeeded by SHEXL 2014 Note

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
48 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
27 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# start Validation Reply Form
    _vrf_RFACR01_hijazi3m
    
    PROBLEM: The value of the weighted R factor is > 0.45
    RESPONSE: ...
    
    _vrf_DIFMX01_hijazi3m
    
    PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
    RESPONSE: ...
    
    _vrf_DIFMX02_hijazi3m
    
    PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
    RESPONSE: ...
    
    _vrf_SHFSU01_hijazi3m
    
    PROBLEM: The absolute value of parameter shift to su ratio > 0.05
    RESPONSE: ...
    
    _vrf_PLAT084_hijazi3m
    
    PROBLEM: High wR2 Value (i.e. > 0.25) .................... 0.47 Report
    RESPONSE: ...
    
    _vrf_PLAT215_hijazi3m
PROBLEM: Disordered C40 has ADP max/min Ratio ..... 5.4 Note

PROBLEM: Large Hirshfeld Difference S2 -- O6 .. 0.40 Ang.

PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of S1 Check

PROBLEM: No (Interpretable) Reflections found in FCF .... Please Check

PROBLEM: Maximum Shift/Error ......................... 0.08 Why ?

PROBLEM: Ratio of Maximum / Minimum Residual Density .... 3.14 Report

PROBLEM: Large Reported Max. (Positive) Residual Density 2.15 eA-3

PROBLEM: Atom S1 has ADP max/min Ratio ..... 3.8 prolat

PROBLEM: Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio

PROBLEM: Hirshfeld Test Diff for C45 -- C46 .. 7.0 s.u.

PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of Co1 Check

PROBLEM: Short C(sp3)-C(sp2) Bond C52 - C54 .. 1.41 Ang.

PROBLEM: Long C(sp2)-C(sp2) Bond C47 - C48 .. 1.56 Ang.
PROBLEM: Structure Contains Solvent Accessible VOIDS of . 46 Ang3

PLATON version of 11/08/2016; check.def file version of 04/08/2016