checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-Sm_hex

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: 3-Sm_hex

```
Bond precision:   C-C = 0.0117 A           Wavelength=1.54178

Cell:           a=11.5391(8)       b=13.1434(9)      c=20.9935(17)
                alpha=85.410(4)    beta=75.777(4)    gamma=67.979(3)
Temperature:    120 K

                Calculated                  Reported
Volume          2860.9(4)                   2860.9(4)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
Moiety formula  C56 H89 O4 P4 Sm            C56 H89 O4 P4 Sm
Sum formula     C56 H89 O4 P4 Sm            C56 H89 O4 P4 Sm
Mr              1100.52                     1100.50
Dx,g cm-3       1.278                       1.278
Z               2                           2
Mu (mm-1)       9.076                       9.076
F000            1158.0                      1158.0
F000'           1152.35
h,k,lmax        14,16,25                    14,16,25
Nref            11400                       11259
Tmin,Tmax       0.332,0.520                 0.286,0.754
Tmin'           0.138

Correction method= # Reported T Limits: Tmin=0.286 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.988            Theta(max)= 72.725

R(reflections)= 0.0741( 9612)                    wR2(reflections)=
                                                 0.2030( 11259)
S = 1.026                  Npar= 785
```

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

PLAT213_ALERT_2_B Atom C43 has ADP max/min Ratio ..... 4.3 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From Sm1 2.84 eA-3

Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.94Ang From Sm1 2.81 eA-3

Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.95Ang From Sm1 -2.53 eA-3

Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

Alert level C

PLAT213_ALERT_2_C Atom Sm1 has ADP max/min Ratio ..... 3.2 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom P4 has ADP max/min Ratio ..... 3.8 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom P3 has ADP max/min Ratio ..... 3.4 oblate

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom O3 has ADP max/min Ratio ..... 3.1 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom O4 has ADP max/min Ratio ..... 3.9 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C29 has ADP max/min Ratio ..... 3.3 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio ..... 3.4 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C32 has ADP max/min Ratio ..... 3.5 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C33 has ADP max/min Ratio ..... 3.6 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C45 has ADP max/min Ratio ..... 3.5 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

PLAT213_ALERT_2_C Atom C46 has ADP max/min Ratio ..... 4.0 prolat

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

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PLAT213_ALERT_2_C Atom C48            has ADP max/min Ratio .....       3.1 prolat
```

Author Response: This is due to the extensive disorder present in the model and overall quality of the dataset.

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.1 Ratio
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         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Sm1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C49 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.7 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01175 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         31 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         41 Report
               -1 14  0,    1 15  0,    1-14  1,    0  1  1,    0  3  1,    0  4  1,
                1  4  1,    0  5  1,    1  7  1,   -1 14  1,    0 14  1,    1 15  1,
                1  6  2,   -1 14  2,    0 14  2,    2 15  2,    0 14  3,    1 14  3,
                2 15  3,    3 15  3,    2  1  4,    1  6  4,    1 13  4,    0 14  4,
                1 14  4,    2 15  4,   -1 -4  5,    0 14  5,    2 15  5,    3 15  5,
              -10 -2  6,    0 14  6,    5 14  9,    5 15  9,    6 15  9,    4 14 10,
                5 14 10,    2 11 16,    6 -1 20,    9  1 20,    9  1 21,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From Sm1              1.93 eA-3
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Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From Sm1              1.71 eA-3
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Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From O2               1.57 eA-3
```

Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Sm1             -2.50 eA-3
```

Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From Sm1           -1.98 eA-3
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Author Response: The residualt density could not be modelled as any chemically sensible species and its presence is due to the proximity of a strong absorber (Sm)

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PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.54Ang From O4      .       0.72 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O3      .       0.58 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         36 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          82 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
              H3A   H2
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      10.32 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0080 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0080 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        28% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H12B     ..H23F     .       2.07 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H17      ..H26C     .       2.11 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H31      ..H41A     .       2.02 Ang.
                                                    x,y,z  =      1_555 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1457 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        100 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.009 Note
              Predicted wR2: Based on SigI**2  6.74 or SHELX Weight 19.79
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  30 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  39 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   5 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 22/08/2024; check.def file version of 21/08/2024

Datablock 3-Sm_hex - ellipsoid plot