checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_Sm_tol

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: 1_Sm_tol

Bond precision: C-C = 0.0075 A Wavelength=1.54178

Cell: a=11.6184(8) b=13.1241(9) c=17.2669(12)
alpha=83.085(3) beta=73.247(3) gamma=65.722(3)
Temperature: 120 K

	Calculated	Reported
Volume	2298.2(3)	2298.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C42 H66 O3 P3 Sm), C7 H8	C42 H66 O3 P3 Sm, 0.5(C7 H8)
Sum formula	C91 H140 O6 P6 Sm2	C45.50 H70 O3 P3 Sm
Mr	1816.57	908.27
Dx,g cm-3	1.313	1.313
Z	1	2
Mu (mm-1)	10.851	10.851
F000	948.0	948.0
F000'	941.35	
h,k,lmax	14,16,21	14,16,21
Nref	9125	9007
Tmin,Tmax	0.257,0.588	0.358,0.754
Tmin'	0.096	

Correction method= # Reported T Limits: Tmin=0.358 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 72.444

R(reflections)= 0.0481(8374) wR2(reflections)= 0.1409(9007)

S = 1.077 Npar= 512

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

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PLAT972_ALERT_2_B Check Calcd Resid. Dens.  0.85Ang From Sm1           -2.53 eA-3
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Author Response: The residual density is due to the proximity of a strong absorber (Sm) and could not be modelled as any chemically sensible species.

Alert level C

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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C42 H66 O3 P3 Sm), C7 H8
             Rep.: C42 H66 O3 P3 Sm, 0.5(C7 H8)
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    2)        3.0 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         35 Report
               13  9  0,  10 13  0, -10-12  3,  -8-13  4, -11-10  4, -10-12  5,
               -9-12  5,  -7-12  5,  -6-12  5,  -8-12  6,  -7-12  6,  -8-10  6,
               -8-12  8,  -8-11  8,  -4 -4  8,  -8-10  9,  -9 -9  9,  -7-11 10,
               -8-10 10,  -8 -8 11,  -8 -7 12,  -5 -9 13,  -4 -9 13,  -5 -8 13,
               -5 -7 13,  -4 -5 13,  -5 -8 14,  -6 -7 14,  -5 -7 14,  -4 -7 14,
               -7 -3 14,  -3 -7 15,  -4 -5 15,  -3 -4 15,   7  8 18,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.96Ang From Sm1             2.50 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.91Ang From Sm1             2.12 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.89Ang From Sm1             1.75 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.86Ang From Sm1             1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.10Ang From Sm1             1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From Sm1            -2.28 eA-3
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Author Response: The residual density is due to the proximity of a strong absorber (Sm) and could not be modelled as any chemically sensible species.

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PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Sm1       1.05 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H36B      .      -0.45 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          4 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms            7 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large        0.11 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records           1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records           1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records           1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records           1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records           1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0080 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............         0.5 Check
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             C43     C44     C45     C46     C47     C48     C49     H44
             H45     H46     H47     H48     H49A    H49B    H49C
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)      7.50 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        15 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sm1       (III)     .      3.05 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers         1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        90 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        83 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         6 Note
             -11-12  3, -10-12  3, -10-12  5,  -9-12  5,  -8-12  6,  -8-11  8,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     3.632 Note
             Predicted wR2: Based on SigI**2  3.88 or SHELX Weight 13.08
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
11 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
11 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 22/08/2024; check.def file version of 21/08/2024

Datablock 1_Sm_tol - ellipsoid plot