checkCIF/PLATON report

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

Bond precision: C-C = 0.0071 A Wavelength=1.54178

Cell: a=16.7184(6) b=24.4547(9) c=16.8001(6)
alpha=90 beta=90.881(2) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	6867.8(4)	6867.8(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C56 H89 O4 P4 Sm), C7 H8 [+ solvent]	C56 H89 O4 P4 Sm, 0.5(C7 H8), 1.5[C7H8]
Sum formula	C119 H186 O8 P8 Sm2 [+ solvent]	C70 H105 O4 P4 Sm
Mr	2293.17	1284.76
Dx,g cm-3	1.109	1.243
Z	2	4
Mu (mm-1)	7.580	7.636
F000	2416.0	2716.0
F000'	2404.91	
h,k,lmax	20,30,20	20,30,20
Nref	13646	13568
Tmin,Tmax	0.276,0.341	0.363,0.754
Tmin'	0.176	

Correction method= # Reported T Limits: Tmin=0.363 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 72.624

R(reflections)= 0.0511(10802)

wR2(reflections)= 0.1351(13568)

S = 1.023 Npar= 662

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

PLAT250_ALERT_2_B Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 4.1 Note

Author Response: This is due to the disorder present in part of the model and the use of restraints to aid refinement.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.24 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report
7 0 3, 6 0 6, 7 1 7, 6 2 8, -12 19 8, 15 12 10,
13 13 11, 12 14 12, 10 16 12, 9 19 12, 15 0 13, 15 1 13,
14 0 14, -7 15 15, -4 8 16, -4 12 16, 0 15 17, 1 15 17,
-3 6 19, -1 9 19, 0 0 20, -2 1 20, 0 1 20,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From Sm1 1.97 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3 . -0.33 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C70 H105 O4 P4 Sm1
Atom count from the _atom_site data: C59.5 H93 O4 P4 Sm1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C70 H105 O4 P4 Sm
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	280.00	238.00	42.00
H	420.00	372.00	48.00
O	16.00	16.00	0.00
P	16.00	16.00	0.00
Sm	4.00	4.00	0.00

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
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H3
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C59.50 H93 O4 P4 Sm
Rep.: C70 H105 O4 P4 Sm

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PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C56 H89 O4 P4 Sm), C7 H8
             Rep.: C56 H89 O4 P4 Sm, 0.5(C7 H8), 1.5[C7H8]
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .       0.73 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      19.06 Why ?
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
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
             C57     C58     C59     C60     C61     C62     C63     H57
             H58     H59     H60     H61     H63A    H63B    H63C
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
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         15 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sm1       (III)     .       3.16 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         47 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         55 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.812 Note
             Predicted wR2: Based on SigI**2  4.80 or SHELX Weight 13.21
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
29 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
13 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_tol - ellipsoid plot