checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b20220721b_0ma

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: mo_b20220721b_0ma

Bond precision: C-C = 0.0045 A Wavelength=0.71073

Cell: a=45.8197(17) b=10.2025(4) c=13.2383(5)
alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	6188.6(4)	6188.6(4)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	2(C72 H74 B N3 O Si), 2(C4 H8 O), C2 H3 N	C72 H74 B N3 O Si, 0.5(C2 H3 N), C4 H8 O
Sum formula	C154 H167 B2 N7 O4 Si2	C77 H82 B N3.50 O2 Si
Mr	2257.75	1127.36
Dx,g cm-3	1.212	1.210
Z	2	4
Mu (mm-1)	0.090	0.090
F000	2420.0	2414.0
F000'	2421.16	
h,k,lmax	63,14,18	63,14,18
Nref	17143[9460]	17094
Tmin,Tmax	0.989,0.993	0.574,0.746
Tmin'	0.989	

Correction method= # Reported T Limits: Tmin=0.574 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.81/1.00 Theta(max)= 29.428

R(reflections)= 0.0513(15059) wR2(reflections)= 0.1337(17094)

S = 1.062 Npar= 758

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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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       3.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of         O1 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of         C1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         C3 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         C5 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         C2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1      0.204 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N1      0.169 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00454 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C1       - C3       .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C1       - C5       .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C3       - C6       .       1.42 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         21 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         10 Note
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C77 H82 B1 N3.5 O2 Si1
            Atom count from _chemical_formula_moiety:C77 H83.5 B1 N3.5 O2 Si1
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:C77 H82 B1 N3.5 O2 Si1
            Atom count from the _atom_site data:  C77 H83.5 B1 N3.5 O2 Si1
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  C77 H82 B N3.50 O2 Si
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         308.00    308.00    0.00
           H         328.00    334.00   -6.00
           B           4.00      4.00    0.00
           N          14.00     14.00    0.00
           O           8.00      8.00    0.00
           Si          4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          5 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
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PLAT300_ALERT_4_G Atom Site Occupancy of H4A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C        Constrained at        0.5 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1       .      108.0 Degree
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          3 Check
PLAT791_ALERT_4_G Model has Chirality at C40         (Sohnke SpGr)         S Verify
PLAT791_ALERT_4_G Model has Chirality at C78         (Sohnke SpGr)         S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        31 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         8 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        12 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         8 Info
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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
 19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 20 ALERT level G = General information/check it is not something unexpected

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 14 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 18/05/2022; check.def file version of 17/05/2022

Datablock mo_b20220721b_0ma - ellipsoid plot