checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Oligomer_4

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: Oligomer_4

Bond precision: C-C = 0.0324 A Wavelength=1.54178

Cell: a=12.5708(14) b=51.249(6) c=12.9887(14)
alpha=90 beta=90.116(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	8367.8(16)	8367.8(16)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	2(C75 H100 Cl5 N17 O22 S5), 2(C5 H5 N), 11(C4 H8 O)	?
Sum formula	C204 H298 Cl10 N36 O55 S10	C102 H149 Cl5 N18 O27.50 S5
Mr	4809.90	2404.93
Dx,g cm-3	0.955	0.954
Z	1	2
Mu (mm-1)	1.835	1.835
F000	2544.0	2544.0
F000’	2558.14	
h,k,lmax	11,46,11	11,46,11
Nref	13226[6720]	12960
Tmin,Tmax	0.820,0.863	0.809,1.000
Tmin’	0.480	

Correction method= # Reported T Limits: Tmin=0.809 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.93/0.98 Theta(max)= 44.531

R(reflections)= 0.1308(8288) wR2(reflections)= 0.3451(12960)

S = 1.254 Npar= 1403

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4549

Author Response: Crystals did not diffract past ca. 1.2A resolution.

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: It was not possible to reliably model heavily disordered solvent molecules in structural voids.

Alert level B

PLAT035_ALERT_1_B	_chemical_absolute_configuration Info Not Given	Please Do !
PLAT049_ALERT_1_B	Calculated Density Less Than 1.0 gcm-3	0.9545 Check
PLAT089_ALERT_3_B	Poor Data / Parameter Ratio (Zmax < 18)	4.73 Note
PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds	0.03241 Ang.
PLAT922_ALERT_1_B	wR2 in the CIF and FCF Differ by	0.0053 Check
PLAT926_ALERT_1_B	Reported and Calculated R1 Differ by	0.0054 Check

Alert level C

PLAT082_ALERT_2_C	High R1 Value	0.13 Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.35 Report
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of	C8_3 Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of	C8_5 Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of	C8_7 Check
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of	C6_9 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C4_3 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C7_3 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C7_5 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C7_7 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C_9 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C_10 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C7_11 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of	C_12 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1 Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Cl10_3	0.112 Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C4_9 -C9_9	1.37 Ang.
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C4_11 -C9_11	1.37 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N_13 --Ha_13 .	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.675 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.455	76 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	9 Check
PLAT921_ALERT_1_C	R1 in the CIF and FCF Differ by	0.0023 Check
PLAT923_ALERT_1_C	S Values in the CIF and FCF Differ by	0.024 Check
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	0.0042 Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement	Please Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 189 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 201 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 13 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.124 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 35 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 40 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of N31_41 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32_41 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H15B_33    Constrained at       0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       5.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       5.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 11  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )       6.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 13  )       3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 14  )       3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 15  )       3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 16  )       3.25 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       Ca_1 Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_23         106.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_24         107.5 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_26         107.4 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_27         108.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_28         104.3 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_31         105.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_22         104.6 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_29         107.4 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_30         107.2 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O11_33         108.7 Degree
PLAT411_ALERT_2_G Short Inter H...H Contact  H8_7     ..H15A_22  .       2.09 Ang.
                                                     x,y,z  =      1_555 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  HaB_9    ..H13A_27  .       2.10 Ang.
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                                                  1+x,y,z  =      1_655 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  HbA_9    ..H13A_27  .       2.09 Ang.
                                                  1+x,y,z  =      1_655 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H5_9     ..H14B_24  .       2.10 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     HaB_1    ..H15A_31  .       2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     HbC_2    ..H12A_32  .       2.10 Ang.
                                                 2-x,1/2+y,1-z  =      2_756 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     HdA_3    ..H13B_30  .       2.12 Ang.
                                                  2-x,1/2+y,-z  =      2_755 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl10_11  ..O_9      .       3.16 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11_28   ..C14_22          2.54 Ang.
                                                    x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11_33   ..C14_23          2.29 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O11_33   ..C15_23          2.63 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14_23   ..C12_33          2.54 Ang.
                                                   x,y,1+z  =      1_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13_27   ..C14_28          3.05 Ang.
                                                  x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C15_28   ..C14_22          3.08 Ang.
                                                    x,y,z  =      1_555 Check
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder          ! Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        415 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
            C5 H5 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
            C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
            C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         11 Note
            C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         12 Note
            C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         15 Note
            C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         16 Note
            C4 H8 O
PLAT791_ALERT_4_G Model has Chirality at Ca_2        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_3        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_4        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_5        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_6        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_7        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_8        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_9        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_10       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_11       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_12       (Chiral SPGR)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2258 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
280 **ALERT level G** = General information/check it is not something unexpected

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 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 47 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
248 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 22/12/2019; check.def file version of 13/12/2019

Datablock Oligomer_4 - ellipsoid plot