checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Oligomer_7

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_7

Bond precision: C-C = 0.0809 A Wavelength=1.54178

Cell: a=17.1947(15) b=17.2126(16) c=35.063(3)
alpha=90 beta=90.043(4) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	10377.4(16)	10377.5(16)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	2(C100 H131 Cl7 N22 O29 S7), 14(C H Cl3), 11(Cl)	?
Sum formula	C214 H276 Cl67 N44 O58 S14	C108.83 H139.83 Cl33.50 N22 O29 S7
Mr	7216.80	3632.20
Dx,g cm-3	1.155	1.162
Z	1	2
Mu (mm-1)	5.130	5.133
F000	3695.0	3721.0
F000’	3732.19	
h,k,lmax	13,13,28	13,13,28
Nref	11133[5869]	9948
Tmin,Tmax	0.567,0.735	0.577,1.000
Tmin’	0.514	

Correction method= # Reported T Limits: Tmin=0.577 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.89 Theta(max)= 38.075

R(reflections)= 0.2096(5200) wR2(reflections)= 0.5270(9948)

S = 1.904 Npar= 1848

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

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_18

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_21

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_21

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_21

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_23

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_29

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_30

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl1_31

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

LABEL01_ALERT_1_A An _atom_site_label occurs more than once in the atom list.
Cl2_31

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue. .

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4000

Author Response: In general the quality of crystals was low possibly due to twinning and large amount of disordered solvent. Crystals did not diffract past ca. 1.3 A resolution.

PLAT070_ALERT_1_A Duplicate Atomic Label on INPUT ..... CL1_21 Note

Author Response: Duplicate labels belong to disordered atoms in Parts 1 and 2 of the same residue.

PLAT082_ALERT_2_A High R1 Value ..... 0.21 Report

Author Response: In general the quality of crystals was low possibly due to twinning and large amount of disordered solvent.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.53 Report

Author Response: In general the quality of crystals was low possibly due to twinning and large amount of disordered solvent.

PLAT089_ALERT_3_A Poor Data / Parameter Ratio (Zmax < 18) ..... 3.08 Note

Author Response: Structure was refined with restraints to offset the effects of overfitting.

PLAT340_ALERT_3_A Low Bond Precision on C-C Bonds ..... 0.0809 Ang.

Author Response: In general the quality of crystals was low possibly due to twinning and large amount of disordered solvent.

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

Author Response: Although many of solvent molecules were included in the model it was still not possible to model heavily disordered content of structural voids.

Alert level B

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PLAT035_ALERT_1_B _chemical_absolute_configuration Info  Not Given     Please Do !
PLAT220_ALERT_2_B NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range       6.1 Ratio
PLAT260_ALERT_2_B Large Average Ueq of Residue Including    Cl1_24      0.364 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including    Cl1_26      0.311 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including    Cl1_27      0.345 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including     Cl_28      0.303 Check
PLAT921_ALERT_1_B R1  in the CIF and FCF Differ by ...............    0.0070 Check
PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by ...............    0.0131 Check
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Alert level C

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.125
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........     0.125 Report
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ    Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..     47.60 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT213_ALERT_2_C Atom N_12            has ADP max/min Ratio .....       3.4 prolat
PLAT213_ALERT_2_C Atom N_16            has ADP max/min Ratio .....       3.4 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1  N   Ueq(max) / Ueq(min) Range       4.8 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1  O   Ueq(max) / Ueq(min) Range       4.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1  S   Ueq(max) / Ueq(min) Range       3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range      7.0 Ratio
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of       C_3 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of      C6_8 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of     C6_12 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of       N_4 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of       C_1 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of      C7_2 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of      C7_4 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of       C_6 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of      C7_8 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of     C7_10 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of     C7_12 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of      C_14 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of     C7_14 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of      C_15 Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of     C1_17 Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of     C1_19 Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of     C1_27 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_2      0.195 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_17      0.212 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_18      0.232 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_19      0.234 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_20      0.198 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_21      0.221 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_22      0.223 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including    Cl1_23      0.269 Check
PLAT420_ALERT_2_C D-H Without Acceptor       N_16     --H0A_16   .    Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.400       181 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .        18 Check
PLAT923_ALERT_1_C S    Values in the CIF and FCF Differ by .......     0.058 Check
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PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 21.02 Check
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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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:C108.83 H139.83 Cl33.5 N22 O29 S
Atom count from the _atom_site data: C107 H138 Cl33.5 N22 O29 S7
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 2
From the CIF: _chemical_formula_sum C108.83 H139.83 Cl33.50 N22 O29 S7
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	217.66	214.00	3.66
H	279.66	276.00	3.66
Cl	67.00	67.00	0.00
N	44.00	44.00	0.00
O	58.00	58.00	0.00
S	14.00	14.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 213 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 220 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 16 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.140 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 33 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 43 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 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 Cl1_18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_21 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_23 Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_24     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_24     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_24     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_24      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_24      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_26     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_26     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_26     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_26      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_26      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_25     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_25     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_25     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_25      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_25      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_31     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2_31     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3_31     Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1_31      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1_31      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl11       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl20       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_21     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5_22     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl28       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl_28      Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl44       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_29     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl45       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1_30     Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl46       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl47       Constrained at       0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       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 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 20  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 21  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 22  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 23  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 24  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 25  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  9  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10  )       2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 12  )       1.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 13  )       1.25 Check
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PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 14  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 15  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 16  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 17  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 18  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 19  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 20  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 21  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 22  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 23  )       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 24  )       0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 25  )       0.25 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       Ca_1 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl2_17   ..O2_8     .       3.15 Ang.
                                                -1+x,y,z  =      1_455 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl2_19   ..O2_10    .       3.04 Ang.
                                              1-x,1/2+y,1-z  =      2_656 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl2_27   ..O2_12    .       2.94 Ang.
                                                1+x,y,z  =      1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl10_2   ..Cd_2             2.92 Ang.
                                               -x,-1/2+y,-z  =      2_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3_21   ..C6_12            2.99 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3_21   ..C5_12            3.02 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3_22   ..C6_12            3.10 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3_22   ..C5_12            3.16 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl3_23   ..C1_17            3.21 Ang.
                                              -x,-1/2+y,1-z  =      2_546 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1_26   ..C_11             3.21 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2_25   ..C1_20            3.19 Ang.
                                               -x,1/2+y,1-z  =      2_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2_31   ..C8_4             3.00 Ang.
                                               -x,-1/2+y,-z  =      2_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2_31   ..C9_4             3.11 Ang.
                                               -x,-1/2+y,-z  =      2_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2_4     ..C1_18            2.83 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3_6     ..C1_27            2.93 Ang.
                                              1-x,1/2+y,1-z  =      2_656 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3_8     ..C1_19            3.01 Ang.
                                                x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3_10    ..C1_17            2.91 Ang.
                                              -x,-1/2+y,1-z  =      2_546 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3_12    ..C1_20            2.98 Ang.
                                                x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl10_2   ..Cl3_31           3.08 Ang.
                                                x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl10_8   ..Cl2_22           3.39 Ang.
                                             1-x,-1/2+y,1-z  =      2_646 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl10_12  ..Cl1_21           3.17 Ang.
                                                x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1_17   ..Cl3_25           2.83 Ang.
                                                x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1_19   ..Cl2_23           2.70 Ang.
                                                x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2_19   ..Cl3_23           3.35 Ang.
                                              1-x,1/2+y,1-z  =      2_656 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........        361 Note
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PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.98000 Dev...       0.02 Ang.
             CB_7     -HB3_7          1.555   1.555 ........     #  132 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.20 Dev...       1.20 Degree
             NT_2    -CB_2    -HB1_2      1.555  1.555  1.555     #   23 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             CA_3    -CB_3    -HB1_3      1.555  1.555  1.555     #   79 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             HB2_3   -CB_3    -HB3_3      1.555  1.555  1.555     #   84 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             HD1_4   -CD_4    -HD2_4      1.555  1.555  1.555     #  114 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             CG_4    -CD_4    -HD3_4      1.555  1.555  1.555     #  115 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             CA_7    -CB_7    -HB1_7      1.555  1.555  1.555     #  229 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             HB2_7   -CB_7    -HB3_7      1.555  1.555  1.555     #  234 Check
PLAT722_ALERT_1_G Angle   Calc      120.00, Rep      118.90 Dev...       1.10 Degree
             CA_9    -N_9     -H0_9       1.555  1.555  1.555     #  303 Check
PLAT722_ALERT_1_G Angle   Calc      105.00, Rep      106.10 Dev...       1.10 Degree
             CD_10   -CG_10   -HG_10      1.555  1.555  1.555     #  332 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             HD1_12  -CD_12   -HD2_12     1.555  1.555  1.555     #  414 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             CG_12   -CD_12   -HD3_12     1.555  1.555  1.555     #  415 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             HD2_12  -CD_12   -HD3_12     1.555  1.555  1.555     #  417 Check
PLAT722_ALERT_1_G Angle   Calc      107.00, Rep      108.10 Dev...       1.10 Degree
             HB1_14  -CB_14   -HB2_14     1.555  1.555  1.555     #  477 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.70 Dev...       1.30 Degree
             CL2_18  -C1_18   -H1_18      1.555  1.555  1.555     #  548 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.90 Dev...       1.10 Degree
             CL2_24  -C1_24   -H1_24      1.555  1.555  1.555     #  583 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         12 Note
             C H Cl3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         15 Note
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         16 Note
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         18 Note
             Cl
PLAT791_ALERT_4_G Model has Chirality at Cg_2        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_3        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_4        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_5        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_6        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_7        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_8        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_9        (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_10       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_11       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_12       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_13       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Cg_14       (Chiral SPGR)          S Verify
PLAT791_ALERT_4_G Model has Chirality at Ca_15       (Chiral SPGR)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       3723 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .      68.34% Note
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PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.31 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)         Est.d BASF       0.49 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1-1 0)         Est.d BASF       0.49 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 1 0)         Est.d BASF       0.48 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          7 Note
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  16 ALERT level A = Most likely a serious problem - resolve or explain
   8 ALERT level B = A potentially serious problem, consider carefully
  43 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 188 ALERT level G = General information/check it is not something unexpected

  38 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  67 ALERT type 2 Indicator that the structure model may be wrong or deficient
  13 ALERT type 3 Indicator that the structure quality may be low
 133 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 22/12/2019; check.def file version of 13/12/2019

Datablock Oligomer_7 - ellipsoid plot