

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Oligomer\_6

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\_6

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Bond precision:	C-C = 0.0142 A	Wavelength=1.54178	
Cell:	a=17.1537(4)	b=17.1537(4)	c=28.9825(8)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	8528.1(5)	8528.1(5)	
Space group	P 41 21 2	P 41 21 2	
Hall group	P 4abw 2nw	P 4abw 2nw	
Moiety formula	2(C25.43 H33.71 C11.71 N5.71 O7.43 S1.71), 3(C H1.50 N0.50), 2(	2.28573 (C89 H118 C16 N20 O26 S6), 20(C2 H3 N)	
Sum formula	C60.86 H82.43 C13.43 N16.43 O14.86 S3.43	C243.43 H329.71 C113.71 N65.71 O59.43 S13.71	
Mr	1513.28	6052.96	
Dx, g cm <sup>-3</sup>	1.179	1.179	
Z	4	1	
Mu (mm <sup>-1</sup> )	2.407	2.406	
F000	3178.2	3178.0	
F000'	3196.62		
h,k,lmax	20,20,35	20,20,34	
Nref	7960[ 4535]	7920	
Tmin,Tmax	0.750,0.749	0.743,1.000	
Tmin'	0.680		

Correction method= # Reported T Limits: Tmin=0.743 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.99      Theta(max)= 69.112

R(reflections)= 0.0985( 5498)      wR2(reflections)= 0.3149( 7920)

S = 1.057      Npar= 503

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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.

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**Alert level B**

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.01417 Ang.

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**Alert level C**

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check  
PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.31 Report  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N37 --C36 . 0.17 Ang.  
PLAT241\_ALERT\_2\_C High MainMol Ueq as Compared to Neighbors of C3 Check  
PLAT241\_ALERT\_2\_C High MainMol Ueq as Compared to Neighbors of C33 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including C118 0.126 Check  
PLAT771\_ALERT\_2\_C Check N-H Bond in CIF: N34 --H33C .. 1.36 Ang.  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 3 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

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**Alert level G**

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: C243.4299 H329.7100 Cl13.71 N  
Atom count from \_chemical\_formula\_moiety:C129 H178 Cl6 N40 O26 S6  
PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 48 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 35 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 11 Report  
PLAT033\_ALERT\_4\_G Flack x Value Deviates > 3.0 \* sigma from Zero . 0.041 Note  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 4.00 Check  
PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 15 Report  
PLAT173\_ALERT\_4\_G The CIF-Embedded .res File Contains DANG Records 30 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 3 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 2 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C118 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C148 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of S9 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of S39 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O10 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O11 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O40 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O41 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of N4 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of N34 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C5 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C6 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C8 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C12 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C13 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C14 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C15 Constrained at 0.8571 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C16 Constrained at 0.8571 Check



PLAT300_ALERT_4_G	Atom Site Occupancy of H70B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H70C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N301	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C302	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C303	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H501	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C502	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C503	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H50A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H50B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H50C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N601	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C602	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C603	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N801	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C802	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C803	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80C	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	57%	Note
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
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C33 ..N501	2.99	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C43 ..N501	3.03	Ang.
		x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....	5	Note
PLAT721_ALERT_1_G	Bond Calc	0.99000, Rep 0.97960 Dev...	0.01	Ang.
	C303 -H30C	1.555 1.555 .....	# 110	Check
PLAT721_ALERT_1_G	Bond Calc	0.99000, Rep 0.97980 Dev...	0.01	Ang.
	C503 -H50B	1.555 1.555 .....	# 119	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	18	Check
	N4 -C3 -H3BE	1.555 1.555 1.555	9.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	19	Check
	C3 -N4 -H3BE	1.555 1.555 1.555	18.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	36	Check
	N7 -C6 -H6B	1.555 1.555 1.555	7.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	42	Check
	C6 -N7 -H6B	1.555 1.555 1.555	5.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	115	Check
	C33 -N34 -H33C	1.555 1.555 1.555	40.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	116	Check
	C33 -N34 -H33D	1.555 1.555 1.555	41.50	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	137	Check
	N37 -C36 -H36A	1.555 1.555 1.555	14.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	142	Check
	C36 -N37 -H36A	1.555 1.555 1.555	9.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF	. #	155	Check
	N34 -S39 -H33D	1.555 1.555 1.555	38.10	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	6	Check

PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	244	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
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	13	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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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  
149 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
11 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
132 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

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**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

