

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 0922_0m

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: 0922_0m

Bond precision: C-C = 0.0048 Å Wavelength=0.71069

Cell: a=17.9031(14) b=18.3379(14) c=32.456(3)
 alpha=90 beta=90 gamma=90

Temperature: 90 K

	Calculated	Reported
Volume	10655.5(15)	10655.3(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C54 H72 O12, C H4 O	C55 H76 O13
Sum formula	C55 H76 O13	C55 H76 O13
Mr	945.16	945.20
Dx, g cm ⁻³	1.178	1.178
Z	8	8
Mu (mm ⁻¹)	0.083	0.083
F000	4080.0	4080.0
F000'	4082.11	
h, k, lmax	21, 21, 38	21, 21, 38
Nref	18829[10232]	18827
Tmin, Tmax	0.963, 0.969	0.963, 0.969
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.963 Tmax=0.969
AbsCorr = MULTI-SCAN

Data completeness= 1.84/1.00 Theta(max)= 25.026

R(reflections)= 0.0415(16621) wR2(reflections)= 0.1116(18827)

S = 1.068 Npar= 1290

Click on the hyperlinks for more details of the test.

 Alert level B

PLAT220_ALERT_2_B	Non-Solvent	Resd	2	C	Ueq(max)/Ueq(min)	Range	7.5	Ratio
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Author Response: There is a large amount of disorder in the structure. In particular some disordered side-chains are severely.

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...	1 Check
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Author Response: The reflection affected by the beam stop was not omitted because it was confirmed that it did not have any influence on the reliability of the final structure.

PLAT934	ALERT 3 B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	7 Check
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Author Response: This alert is originated from insufficient modeling of the disordered alkyl chain.

- Alert level c

PLAT220_ALERT_2_C	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	5.2	Ratio
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Author Response: There is a large amount of disorder in the structure. In particular some disordered side-chains are severely.

PLAT222_ALERT_3_C	Non-Solv. Resd 1	H	Uiso(max)/Uiso(min) Range	5.2	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 2	H	Uiso(max)/Uiso(min) Range	6.7	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C34	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C35	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		025	0.079	Check
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.00484	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C35 - C36	1.42	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H56	..H71	1.96	Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H65	..H68	1.99	Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H2	..H17	1.99	Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H11	..H14	1.97	Ang.
			x,y,z =	1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=		0.595	2	Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.73A	From 025	-0.44	eA-3

- Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.

From the CIF: _publ_requested_category CH00SE FI FM FO CI CM CO or

From the CIF: _chemical_formula_sum:C55 H76 O13

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	13	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C105 --C106 .	10.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C105 --C112 .	5.5	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6%	Note
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C55 -C72 .	1.44	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C1 -C18 .	1.44	Ang.
PLAT791_ALERT_4_G	Model has Chirality at C21 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C27 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C33 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C39 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C45 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C51 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C75 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C81 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C87 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C93 (Chiral SPGR)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C99 (Chiral SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	139	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI	Please	Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	69%	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
14 **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

4 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
18 **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
14 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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.

