

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Form_1_23mbb_sadhna18_ns18_bilpyether

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: Form_1_23mbb_sadhna18_ns18_bilpyether

Bond precision: = 0.0000 A

Wavelength=0.71073

Cell: a=11.6630 (7) b=15.3457 (8) c=17.2204 (10)
 alpha=73.515 (2) beta=81.274 (3) gamma=82.823 (3)
Temperature: 173 K

	Calculated	Reported
Volume	2910.2 (3)	2910.2 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H36 N4 O6	C33 H36 N4 O6
Sum formula	C33 H36 N4 O6	C33 H36 N4 O6
Mr	584.66	584.66
Dx, g cm ⁻³	1.334	1.334
Z	4	4
Mu (mm ⁻¹)	0.093	0.093
F000	1240.0	1240.0
F000'	1240.57	
h, k, lmax	13, 18, 20	13, 18, 20
Nref	10256	10254
Tmin, Tmax	0.983, 0.986	0.630, 0.745
Tmin'	0.979	

Correction method= # Reported T Limits: Tmin=0.630 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta (max)= 24.999

R(reflections)= 0.0851 (6779)

wR2(reflections)=
0.2681 (10254)

S = 1.084

Npar= 1519

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 B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.75 Note

Author Response: In the asymmetric unit, there are two fully disordered molecules, which means there are a lot of parameters to solve. Additionally, the crystal didn't diffract strongly, resulting in a lack of data.

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.27 Report
PLAT213_ALERT_2_C Atom C32A has ADP max/min Ratio 3.1 prolat
PLAT213_ALERT_2_C Atom C62A has ADP max/min Ratio 3.9 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C2 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O11 --C49 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C61 --C62 . 0.19 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 2.3 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 07 0.102 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 01A 0.114 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.022 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 86 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 86 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 24 Report
H1 H2 H3 H3A H4 H6 H5 H6B H7 H8B H9
H12 H3AA H2AA H3AB H4A H6A H1AC H5A H9A H6AA H7AD
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par 0.0050 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par 0.0050 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par 0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar 0.0020 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C31 --C32 . 5.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C34 --C35 . 5.9 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C65 . 7.7 s.u.
PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 100% Note

PLAT301_ALERT_3_G	Main Residue Disorder(Resd	3)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd	4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd	2)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd	1)	63.75	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd	2)	65.41	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd	3)	15.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd	4)	13.59	Check
PLAT309_ALERT_2_G	Single Bonded Oxygen (C-O > 1.3 Ang)		O4A	Check
PLAT309_ALERT_2_G	Single Bonded Oxygen (C-O > 1.3 Ang)		O10A	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C7	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C13	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C25	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C33	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C40	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C46	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C58	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C66	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		13	Note
	H3AA H2AA H3AB H1AA H1AB H2AB H1AC H7AA				
	H7AB H7AC H6AA H7AD H8AA				
PLAT721_ALERT_1_G	Bond Calc	0.85000, Rep	0.84000 Dev...	0.01	Ang.
	O9A -H9A	1_555 1_555	# 249	Check
PLAT722_ALERT_1_G	Angle Calc	106.00, Rep	107.10 Dev...	1.10	Degree
	C61A -C64A -H64C	1_555 1_555 1_555		# 549	Check
PLAT725_ALERT_2_G	D-H Calc	0.85000, Rep	0.84000 Dev...	0.01	Ang.
	O9A -H9A	1_555 1_555	# 19	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C29A	--C33A		1.76	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C62A	--C66A		1.76	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1355	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still			30%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			2	Note
	0 1 0, 0 0 1,				
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			1	Note
	0 1 0,				
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..			50.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		3.72	Note
	Predicted wR2: Based on SigI**2	7.21 or SHELX Weight	26.79		

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
50 **ALERT level G** = General information/check it is not something unexpected

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

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