

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_10598_auto

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: exp_10598_auto

Bond precision: C-C = 0.0024 Å Wavelength=1.54184

Cell: a=9.1546(1) b=15.8727(2) c=17.7781(2)
 alpha=82.390(1) beta=86.872(1) gamma=87.372(1)
Temperature: 296 K

	Calculated	Reported
Volume	2554.79(5)	2554.79(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C61 H43 N3 [+ solvent]	C61 H43 N3
Sum formula	C61 H43 N3 [+ solvent]	C61 H43 N3
Mr	817.98	817.98
Dx, g cm ⁻³	1.063	1.063
Z	2	2
Mu (mm ⁻¹)	0.472	0.472
F000	860.0	860.0
F000'	862.26	
h, k, lmax	11, 20, 22	11, 20, 22
Nref	10933	10450
Tmin, Tmax	0.954, 0.954	0.879, 1.000
Tmin'	0.954	

Correction method= # Reported T Limits: Tmin=0.879 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.956 Theta(max)= 77.929

R(reflections)= 0.0532(8635)	wR2(reflections)=
S = 1.056	0.1726(10450)
Npar= 604	

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 C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.69 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C01Q --C01R . 5.3 s.u.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.208 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 19 Report
-1 1 0, -9 -8 7, -8 10 9, -3 17 9, 2 18 9, 7 13 11,
-7 10 12, -2-13 13, 2-13 13, 8 -5 13, 8 -4 13, 8 -3 13,
-3 15 13, 8 -3 14, 8 -2 14, 8 3 14, 7 -4 15, 7 -3 16,
7 1 17,



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 64 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0200 Report
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C006 -C00H . 1.44 Ang.
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 107 Note
N001 N002 N003 C004 C005 C006 C007 C008
C009 C00A C00B C00C C00D C00E C00F C00G
C00H C00I H00I C00J C00K H00K C00L C00M
C00N H00N C00O C00P C00Q H00Q C00R H00R
C00S H00S C00T H00T C00U H00U C00V C00W
C00X H00X C00Y C00Z H00Z C010 C011 H011
C012 H012 C013 C014 H014 C015 C016 H016
C017 H017 C018 C019 H019 C01A H01A C01B
C01C H01C C01D H01D C01E H01E C01F H01F
C01G H01G C01H H01H C01I C01J C01K H01B
H01I H01J C01L H01L C01M H01M C01N H01K
H01N H01O C01O H01P C01P H01Q H01R H01S
C01Q H01T C01R H01U C01S H015 H00J H00Y
H01V H01W H01X
PLAT860_ALERT_3_G Number of Least-Squares Restraints 193 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 463 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
-1 1 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.14 Note
Predicted wR2: Based on SigI**2 4.17 or SHELX Weight 16.84
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 9 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
5 ALERT type 4 Improvement, methodology, query or suggestion
2 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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