

checkCIF (full publication check) running

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

[Structure factor report](#)

Datablock: I

Bond precision:	C-C = 0.0068 Å	Wavelength=1.54184
Cell:	a=11.7717(4) b=28.966(1) c=16.9134(4)	
	alpha=90 beta=91.318(2) gamma=90	
Temperature: 150 K		

	Calculated	Reported
Volume	5765.6(3)	5765.6(3)
Space group	P n	P 1 n 1
Hall group	P -2yac	P -2yac
Moiety formula	C66 H75 N3, C65 H72 N3, C H3	2(C66 H75 N3), 2 C6 H14
Sum formula	C132 H150 N6	C138 H164 N6
Mr	1820.58	1906.75
Dx, g cm ⁻³	1.049	1.098
Z	2	2
Mu (mm ⁻¹)	0.451	0.470
F000	1968.0	2068.0
F000'	1972.86	
h,k,lmax	14,36,21	14,35,21
Nref	24270[12153]	15430
Tmin,Tmax	0.909,0.978	0.690,1.000
Tmin'	0.909	

Correction method= # Reported T Limits: Tmin=0.690 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.27/0.64 Theta(max)= 76.650

R(reflections)= 0.0759(12872) wR2(reflections)= 0.2305(15430)

S = 1.058 Npar= 1247

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C121 -- C122 .. 7.2 su
 PLAT234_ALERT_4_B Large Hirshfeld Difference C57 -- C58B .. 0.30 Ang.
 PLAT234_ALERT_4_B Large Hirshfeld Difference C57 -- C58A .. 0.28 Ang.
 PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C56 - C57 .. 1.33 Ang.
 PLAT410_ALERT_2_B Short Intra H...H Contact H22 .. H43B .. 1.89 Ang.
 PLAT410_ALERT_2_B Short Intra H...H Contact H56A .. H57A .. 1.80 Ang.
 PLAT915_ALERT_3_B Low Friedel Pair Coverage 30 %

● Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
 calculated from the _atom_site* data lies outside
 the range 0.99 <> 1.01

From the CIF: _cell_formula_units_Z	2
From the CIF: _chemical_formula_weight	1906.75

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	132.00	1585.45
H	1.01	150.00	151.20

N 14.01 6.00 84.04
 Calculated formula weight 1820.69
 STRVA01_ALERT_4_C Flack test results are meaningless.
 From the CIF: _refine_ls_abs_structure_Flack 0.100
 From the CIF: _refine_ls_abs_structure_Flack_su 0.800
 PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
 PLAT213_ALERT_2_C Atom N6 has ADP max/min Ratio 3.4 prolat
 PLAT213_ALERT_2_C Atom C106 has ADP max/min Ratio 3.5 prolat
 PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.4 Ratio
 PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.8 Ratio
 PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 5.7 Ratio
 PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 4.4 Ratio
 PLAT234_ALERT_4_C Large Hirshfeld Difference C45 -- C46 .. 0.16 Ang.
And 2 other PLAT234 Alerts
 More ...
 PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C57 Check
 PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C45 Check
And 3 other PLAT242 Alerts
 More ...
 PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0068 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C65 - C66 .. 1.42 Ang.
 PLAT410_ALERT_2_C Short Intra H...H Contact H13 .. H63B .. 1.98 Ang.
And 3 other PLAT410 Alerts
 More ...
 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 39 Report
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) . 1 Check

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: C138 H164 N6
 Atom count from _chemical_formula_moiety: C144 H178 N6
 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: C138 H164 N6
 Atom count from the _atom_site data: C132 H150 N6
 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 C138 H164 N6
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	276.00	264.00	12.00
H	328.00	300.00	28.00
N	12.00	12.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
 PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
 PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.800 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT044_ALERT_1_G Calculated and Reported Density Dx Differ by .. 0.0493 Check
 PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.14 Report
 PLAT301_ALERT_3_G Main Residue Disorder Percentage = 1 Note
 PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C56 Check
 PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C123 Check
 PLAT344_ALERT_2_G Unusual sp? Angle Range in Solvent/Ion for . C124 Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact C122 .. C124 .. 2.60 Ang.
 PLAT432_ALERT_2_G Short Inter X...Y Contact C123 .. C124 .. 1.77 Ang.
 PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
 PLAT773_ALERT_2_G Check long C-C Bond in CIF: C123 -- C124 . 1.77 Ang.
 PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
 C H3
 PLAT792_ALERT_1_G The Model has Chirality at C85 (Polar SPGR) S Verify
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note
 PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 1 Report
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 243 Note
 PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

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

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

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

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

28 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

11 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

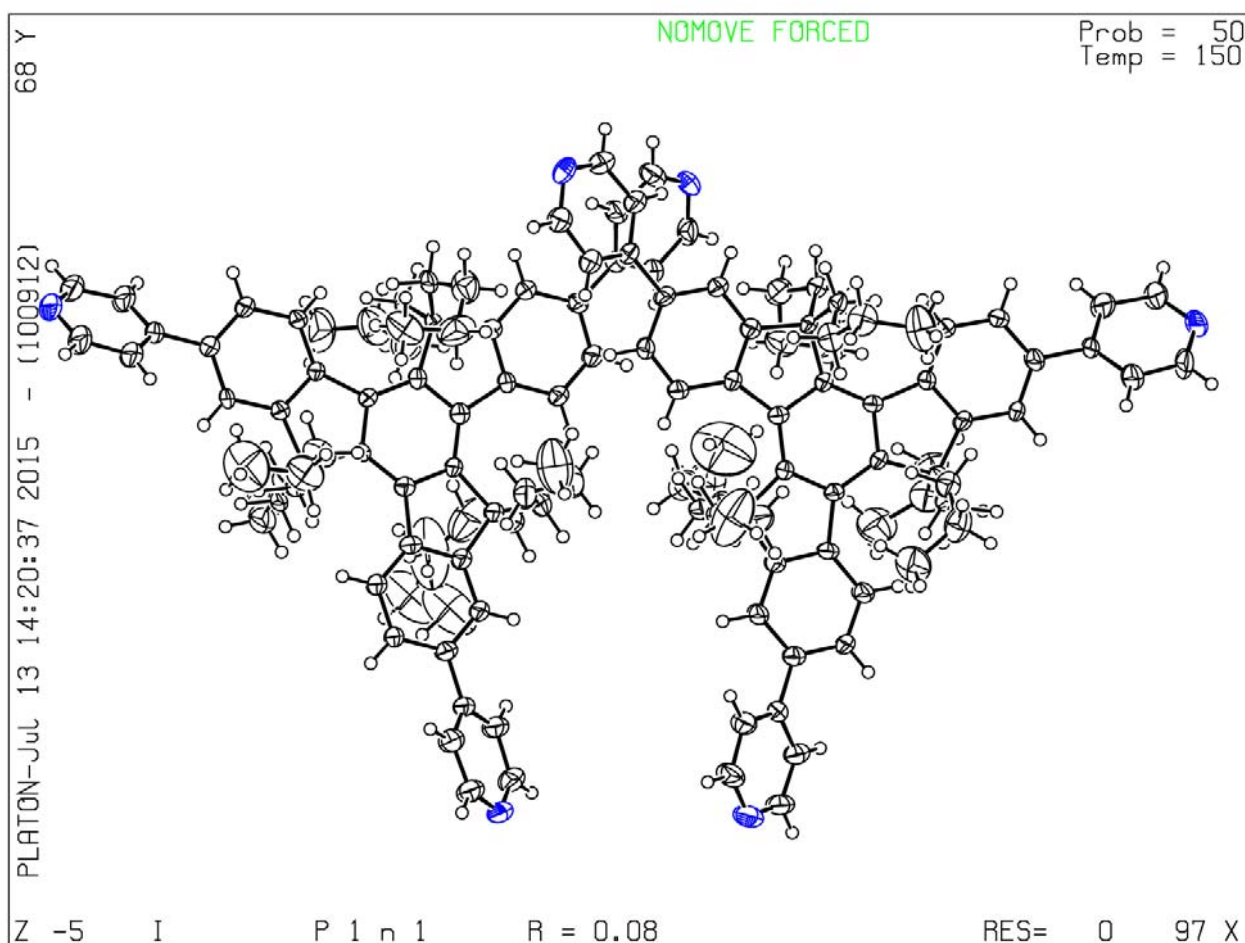
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock I - ellipsoid plot



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