



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_6350

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_6350

Bond precision: C-C = 0.0700 Å

Wavelength=0.02510

Cell: a=8.6(4) b=19.9(3) c=17.9(3)

 alpha=90 beta=99.2(12) gamma=90

Temperature: 97 K

	Calculated	Reported
Volume	3024(157)	3014(174)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C72 H56 N8 O8 [+ solvent]	C18 H14 N2 O2
Sum formula	C72 H56 N8 O8 [+ solvent]	C18 H14 N2 O2
Mr	1161.25	290.32
Dx, g cm ⁻³	1.280	1.280
Z	2	8
Mu (mm ⁻¹)	0.000	0.000
F000	0.0	488.0
F000'	1215.78	
h, k, lmax	8, 19, 17	7, 19, 17
Nref	1550	1169
Tmin, Tmax		0.725, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.725 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.754

Theta (max)= 0.712

R(reflections)= 0.2269(402)

wR2(reflections)=
0.5806(1169)

S = 1.474

Npar= 59

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 A

ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.

Author Response: The quality of the electron diffraction data is sufficient for structure solution, but it is not adequate for the anisotropic refinement of atomic positions.

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4951

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal and the crystals diffract very weakly on the high angle.

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.758 Why?

Author Response: The data were collected using three-dimensional electron diffraction technology, thus the collection angles were limited.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.58 Report

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

 Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.181

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

PLAT020_ALERT_3_B The Reported Value of Rint is Greater Than 0.12 0.181 Report

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 34% Check

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal and the crystals diffract very weakly on the high angle.

PLAT082_ALERT_2_B High R1 Value 0.23 Report

Author Response: The data were collected using three-dimensional electron diffraction technology on only one crystal. Higher R factors are expected due to the strong interaction of electrons.

PLAT149_ALERT_3_B s.u. on the beta Angle is Too Large 1.20 Degree

Author Response: The data were collected through three-dimensional electron diffraction technology, thus the number of collected diffraction spots was limited.

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) Occ>0.5 22 Report

O1	O00I	N003	N008	C1	C001	C002	C005
C007	C009	C00A	C00E	C00D	C00F	C00C	C006
C00H	C00K	C00J	C00B	C00G	C00L		

Author Response: The quality of the electron diffraction data is sufficient for structure solution, but it is not adequate for the anisotropic refinement of atomic positions.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.07 Ang.

Author Response: The data were collected through three-dimensional electron diffraction technology without accounting for dynamical effects. No action taken.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.494 343 Report

2	0	0,	4	0	0,	6	0	0,	1	1	0,	3	1	0,	5	1	0,
7	1	0,	2	2	0,	4	2	0,	6	2	0,	3	3	0,	5	3	0,
7	3	0,	4	4	0,	6	4	0,	5	5	0,	7	5	0,	0	6	0,
6	6	0,	7	7	0,	0	10	0,	-7	1	1,	-5	1	1,	-3	1	1,
-1	1	1,	3	1	1,	5	1	1,	7	1	1,	-6	2	1,	-4	2	1,

(313 More NOT listed: see .ckf listing file)

Author Response: The data were collected through three-dimensional electron diffraction technology, thus the number of collected diffraction spots was limited.

Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

dull

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

whiteish

PLAT148_ALERT_3_C	s.u. on the	a	- Axis is (Too) Large	0.400 Ang.
PLAT148_ALERT_3_C	s.u. on the	b	- Axis is (Too) Large	0.3000 Ang.
PLAT148_ALERT_3_C	s.u. on the	c	- Axis is (Too) Large	0.300 Ang.
PLAT241_ALERT_2_C	High MainResAtom	Ueq	as Compared to Neighbours	C001 Check
PLAT241_ALERT_2_C	High MainResAtom	Ueq	as Compared to Neighbours	C00E Check
PLAT241_ALERT_2_C	High MainResAtom	Ueq	as Compared to Neighbours	C006 Check
PLAT242_ALERT_2_C	Low MainResAtom	Ueq	as Compared to Neighbours	N003 Check
PLAT242_ALERT_2_C	Low MainResAtom	Ueq	as Compared to Neighbours	C00A Check
PLAT353_ALERT_3_C	Long N-H (N0.87,N1.01A)	N003	- H003	1.03 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C001	- C005	1.53 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C00F	- C00F_a	1.53 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			30.332 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			7.439 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..			1 Check
	0 8 0,			

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report

H003

PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check

Calc: C72 H56 N8 O8

Rep.: C18 H14 N2 O2

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C72 H56 N8 O8

Rep.: C18 H14 N2 O2

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250 Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20 Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-17 Units
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C00A	3.47 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C00D	5.78 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C00F	6.09 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C006	3.09 Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	9 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0010 Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	33 Note
	C001 C002 H002 N003 H003 C005 C007 H007	

N008	C009	C00A	C00E	H00E	C00D	H00D	C00F
C00C	H00C	C006	H006	C00H	H00H	C00K	H00K
C00J	H00J	C00B	H00B	C00G	O00I	C00L	H00A
H00F							

PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data 4 Note
 PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 2 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 14 Note
 PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
 PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .. 67.80% Note
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
 0 6 0, 0 10 0,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.1 Low
 PLAT948_ALERT_5_G Externally Supplied Scattering Factors RES 4 Note
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.325 Note
 Predicted wR2: Based on SigI**2 17.46 or SHELX Weight 39.38 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
 19 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 4 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

