



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a

Bond precision:	C-C = 0.0170 Å	Wavelength=0.02510	
Cell:	a=24.618 (7)	b=14.9679 (12)	c=7.3420 (11)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	2705.4 (9)	2705.4 (9)	
Space group	P c c m	P c c m	
Hall group	-P 2 2c	-P 2 2c	
Moiety formula	C36 H28 N2 O [+ solvent]	2 (C36 H28 N2 O)	
Sum formula	C36 H28 N2 O [+ solvent]	C36 H28 N2 O	
Mr	504.60	504.63	
Dx, g cm-3	1.239	1.239	
Z	4	4	
Mu (mm-1)	0.000	0.000	
F000	0.0	446.0	
F000'	1063.83		
h, k, lmax	30, 18, 9	27, 18, 9	
Nref	3000	2494	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.831

Theta(max)= 0.898

R(reflections)= 0.2322(1195)

wR2(reflections)=
0.5747(2494)

S = 0.892

Npar= 104

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.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.57 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.

PLAT411_ALERT_2_A Short Inter H...H Contact H3 ..H3 . 0.96 Ang.
1-x,y,1/2-z = 3_655 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

PLAT411_ALERT_2_A Short Inter H...H Contact H9 ..H17 . 1.25 Ang.
1-x,y,3/2-z = 3_656 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

PLAT411_ALERT_2_A Short Inter H...H Contact H19 ..H19 . 0.92 Ang.
x,1-y,1/2-z = 4_565 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

 Alert level B

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.

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) Occ>0.5 31 Report

O14	N00B	N20	C1	C00A	C2	C001	C3
C002	C4	C003	C5	C007	C6	C008	C7
C009	C8	C9	C10	C11	C12	C13	C15
C16	C17	C18	C19	C21	C22	C23	

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.

PLAT411_ALERT_2_B Short Inter H...H Contact H7 ..H16 . 1.81 Ang.
1-x,y,3/2-z = 3_656 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

PLAT411_ALERT_2_B Short Inter H...H Contact H9 ..H16 . 1.83 Ang.
1-x,y,3/2-z = 3_656 Check

Author Response: This abnormally short intermolecular H...H contact is caused by the initial automatic hydrogenation in Olex2, which only calculates intramolecular bonding geometry without considering the steric repulsion between symmetry- related molecules in the unit cell.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 431 Report

2	0	0,	2	1	0,	3	0	0,	3	1	0,	4	0	0,	4	1	0,
4	2	0,	5	0	0,	5	1	0,	5	2	0,	6	0	0,	6	1	0,
6	2	0,	6	3	0,	7	0	0,	7	1	0,	7	2	0,	7	3	0,
8	0	0,	8	1	0,	8	2	0,	8	3	0,	8	4	0,	9	0	0,
9	1	0,	9	2	0,	9	3	0,	9	4	0,	10	0	0,	10	1	0,

(401 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.

PLAT921_ALERT_1_B R1 in CIF and R1 Calcd from FCF Data Differ by . -0.0204 Check

Author Response: The discrepancies in R1 and wR2 are likely associated with the treatment of the empirical extinction correction in the SHELXL refinement and FCF output. The refinement used electron scattering factors together with an EXTI correction. As noted in the IUCr documentation for PLAT921, SHELXL exports extinction-corrected observed intensities to the FCF. This reflection-dependent transformation may lead to differences between the residuals reported for the refinement and those recalculated from the FCF, including differences associated with the weighting scheme for wR2.

PLAT922_ALERT_1_B wR2 in the CIF and FCF Differ by -0.0171 Check

Author Response: The discrepancies in R1 and wR2 are likely associated with the treatment of the empirical extinction correction in the SHELXL refinement and FCF output. The refinement used electron scattering factors together with an EXTI correction. As noted in the IUCr documentation for PLAT921, SHELXL exports extinction-corrected observed intensities to the FCF. This reflection-dependent transformation may lead to differences between the residuals reported for the refinement and those recalculated from the FCF, including differences associated with the weighting scheme for wR2.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	48% Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	O14 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	N00B Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C3 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C6 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C7 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C8 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C9 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C16 Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C19 Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C00A Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C002 Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C003 Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C008 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01702 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H8 ..H17 .	1.95 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H8 ..H17 .	1.95 Ang.
	x,y,1-z =	6_556 Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N20 --H20A .	Please Check

PLAT420_ALERT_2_C	D-H Bond Without Acceptor N20 --H2OB .	Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-1.234 Report
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.096 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.188 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.038 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.251 Check
PLAT923_ALERT_1_C	S Values in the CIF and FCF Differ by	-0.051 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: C36 H28 N2 O1
 Atom count from _chemical_formula_moiety: C72 H56 N4 O2

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	1 Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	31 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report

H20A H20B

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: C36 H28 N2 O	
	Rep.: 2(C36 H28 N2 O)	

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.50 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at	0.5 Check

H1A H1B H1C H20A H20B

PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C00A Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C3 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C002 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C003 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C6 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C008 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C7 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C9 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C13 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C16 Check
PLAT343_ALERT_2_G	Unusual	Angle Range in Main Residue for	C17 Check

PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C00A	- C19	.	1.51 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C00A	- C19_e	.	1.51 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C3	- C3_e	.	1.70 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C002	- C22	.	1.50 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C6	- C6_e	.	1.75 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C6	- C7_e	.	1.57 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C9	- C13_e	.	1.57 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C13	- C13_e	.	1.66 Ang.
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H1A	..H11	.	2.10 Ang.	

x,y,z =

PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Crystal Structure	1_555 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	9 Note

N00B C00A C001 H001 C002 C003 C007 C008
 C009

PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data	4	Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...	22.50	Deg.
H20A -N20 -H20A 1_555 1_555 6_556 #	3	Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #	19	Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers	7	Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints	35	Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta (Min) [Deg]=	0.05	Note
1 0 0,		
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	22	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	3.8	Low
PLAT948_ALERT_5_G Externally Supplied Scattering Factors RES	4	Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ	3	Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ	3	Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	5.400	Note
Predicted wR2: Based on SigI**2 10.96 or SHELX Weight 62.74		Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0	Info

5 **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
49 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
48 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
5 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

Datablock a - ellipsoid plot

