



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 = 0.0195 Å		Wavelength=0.02510
Cell:	a=29.330 (14)	b=14.8291 (17)	c=7.5004 (14)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3262.2 (17)	3262.2 (17)	
Space group	P c c m	P c c m	
Hall group	-P 2 2c	-P 2 2c	
Moiety formula	C157.33 N8 O4 [+ solvent]	0.5 (C77.33 N4 O2)	
Sum formula	C157.33 N8 O4 [+ solvent]	C38.67 N2 O	
Mr	2065.66	508.45	
Dx, g cm-3	1.051	1.035	
Z	1	4	
Mu (mm-1)	0.000	0.000	
F000	0.0	413.0	
F000'	1031.83		
h, k, lmax	32, 16, 8	25, 15, 8	
Nref	2485	1655	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.666

Theta (max)= 0.790

R(reflections)= 0.3125(981)

wR2(reflections)=
0.6996(1655)

S = 0.990

Npar= 78

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 = 0.5493

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 _diffn_measured_fraction_theta_full value Low . 0.666 Why?

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

PLAT082_ALERT_2_A High R1 Value 0.31 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.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.70 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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) Occ>0.5 33 Report

O1	N6	N12	C1	C00A	C2	C00B	C3
C001	C4	C002	C5	C003	C6	C004	C7
C006	C8	C005	C9	C008	C10	C007	C11
C12	C13	C15	C17	C18	C31	C44	C50
C73							

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.

PLAT241_ALERT_2_B High MainResAtom Ueq as Compared to Neighbours C15 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT242_ALERT_2_B Low MainResAtom Ueq as Compared to Neighbours C7 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.549 659 Report

0	15	0,	1	1	0,	1	15	0,	2	0	0,	2	1	0,	2	2	0,
2	15	0,	3	0	0,	3	1	0,	3	2	0,	3	3	0,	3	15	0,
4	0	0,	4	1	0,	4	2	0,	4	3	0,	4	4	0,	4	15	0,
5	0	0,	5	1	0,	5	2	0,	5	3	0,	5	4	0,	5	5	0,
5	15	0,	6	0	0,	6	1	0,	6	2	0,	6	3	0,	6	4	0,

(629 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 . -0.0226 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

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.

orangish

DIFMX02_ALERT_1_C The maximum difference density is $> 0.1 \times Z_{\text{MAX}} \times 0.75$

The relevant atom site should be identified.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C00A Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C2 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C3 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C4 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C5 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C6 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C8 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C9 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C13 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C18 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours N12 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C008 Check

Author Response: The data were collected through three-dimensional electron diffraction technology. ISOR, DELU and SIMU were used to constrain the atom, but it is not success.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.01947 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4	Please Do
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	35.647 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	8.401 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	16.617 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.546 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.256 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.771 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.986 Check
PLAT922_ALERT_1_C wR2 in the CIF and FCF Differ by	-0.0049 Check

PLAT923_ALERT_1_C S Values in the CIF and FCF Differ by -0.063 Check

Alert level G

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: C38.67 N2 O1

Atom count from the _atom_site data: C40.33340 N2 O1

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

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 4

From the CIF: _chemical_formula_sum C38.67 N2 O

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	154.68	161.33	-6.65
N	8.00	8.00	0.00
O	4.00	4.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	34	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
	Calc: C157.33 N8 O4		
	Rep.: C38.67 N2 O		
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
	Calc: C157.33 N8 O4		
	Rep.: 0.5(C77.33 N4 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	0.70	Report
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C73	4.20	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C31	3.56	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C17	3.95	Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C005	3.91	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	14	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	6	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	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
	C009		
PLAT300_ALERT_4_G	Atom Site Occupancy of C007 Constrained at	0.6667	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)	6%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1	108.6	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C18	2.51	Ang.
	1-x,y,-1/2+z =	8_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C3 ..C15	3.01	Ang.
	1-x,y,1/2+z =	8_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4 ..C4	2.74	Ang.
	x,1-y,3/2-z =	4_566	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C9 ..C9	2.83	Ang.
	1-x,y,3/2-z =	3_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C15 ..C18	2.65	Ang.

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1-x,y,-1/2+z = 8_655 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Crystal Structure ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 11 Note
      C00A      C00B      C001      C002      C003      C004      C006      C005
      C008      C007      C009
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.85 Ratio
PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data 3 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2 --C9 1.81 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C9 --C2 1.81 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4 --C15 1.82 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15 --C4 1.82 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 88 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta (Min) [Deg]= 0.05 Note
      1 0 0,
PLAT948_ALERT_5_G Externally Supplied Scattering Factors RES 3 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 7 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 7 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 7.287 Note
      Predicted wR2: Based on SigI**2 9.67 or SHELX Weight 66.91 Note

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
30 ALERT type 2 Indicator that the structure model may be wrong or deficient
15 ALERT type 3 Indicator that the structure quality may be low
15 ALERT type 4 Improvement, methodology, query or suggestion
4 ALERT type 5 Informative message, check

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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

