



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) b

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: b

Bond precision: C-C = 0.0733 Å

Wavelength=0.02510

Cell: a=46.7 (7) b=9.8 (2) c=8.3 (4)
 alpha=90 beta=94.2 (4) gamma=90
Temperature: 97 K

	Calculated	Reported
Volume	3788 (206)	3788 (206)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C25 H18 N2 O2 [+ solvent]	C25 H18 N2 O2
Sum formula	C25 H18 N2 O2 [+ solvent]	C25 H17 N2 O2
Mr	378.41	377.42
Dx, g cm ⁻³	1.330	1.323
Z	8	8
Mu (mm ⁻¹)	0.000	0.000
F000	0.0	641.0
F000'	1583.74	
h, k, lmax	45, 9, 8	34, 9, 8
Nref	1875	1092
Tmin, Tmax		0.266, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.266 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.582

Theta (max)= 0.705

R(reflections)= 0.2407(521)

wR2(reflections)=
0.6523(1092)

S = 1.110

Npar= 84

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 = 0.4902

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 . 0.583 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) 0.65 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

PLAT082_ALERT_2_B High R1 Value 0.24 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 0.40 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 29 Report
O014 O8 N001 N2 C1 C004 C2 C006
C3 C007 C4 C009 C00J C6 C002 C00A
C8 C00B C00C C00I C11 C00K C12 C14
C19 C22 C27 C35 C37

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 0.07333 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= 0.490 623 Report
6 0 0, 7 1 0, 8 0 0, 9 1 0, 10 0 0, 11 1 0,
12 0 0, 12 2 0, 13 1 0, 14 0 0, 14 2 0, 15 1 0,
16 0 0, 16 2 0, 17 1 0, 18 0 0, 18 2 0, 19 1 0,
19 3 0, 20 0 0, 20 2 0, 21 1 0, 21 3 0, 22 0 0,
22 2 0, 23 1 0, 23 3 0, 24 0 0, 24 2 0, 24 4 0,
(593 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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.140

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_C	The Reported Value of Rint is Greater Than	0.12	0.140	Report
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..		48%	Check
PLAT148_ALERT_3_C	s.u. on the a - Axis is (Too) Large		0.700	Ang.
PLAT148_ALERT_3_C	s.u. on the b - Axis is (Too) Large		0.2000	Ang.
PLAT148_ALERT_3_C	s.u. on the c - Axis is (Too) Large		0.400	Ang.
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours		C00J	Check
PLAT353_ALERT_3_C	Long N-H (N0.87,N1.01A) N2 - H2 .		1.05	Ang.
PLAT362_ALERT_2_C	Short C(sp3)-C(sp2) Bond C8 - C14 .		1.37	Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H009 ..H00C .		2.02	Ang.
	x,1-y,1/2+z =		6_566	Check
PLAT411_ALERT_2_C	Short Inter H...H Contact H00I ..H27 .		2.14	Ang.
	1/2-x,1/2+y,1/2-z =		4_555	Check
PLAT411_ALERT_2_C	Short Inter H...H Contact H22 ..H37 .		2.13	Ang.
	1/2-x,1/2+y,1/2-z =		4_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		43.761	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		8.908	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		11.022	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: C25 H17 N2 O2
 Atom count from _chemical_formula_moiety: C25 H18 N2 O2

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: C25 H17 N2 O2
 Atom count from the _atom_site data: C25 H18 N2 O2

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 8
 From the CIF: _chemical_formula_sum C25 H17 N2 O2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	200.00	200.00	0.00
H	136.00	144.00	-8.00
N	16.00	16.00	0.00
O	16.00	16.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
	H2		
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please	Check
	Calc: C25 H18 N2 O2		
	Rep.: C25 H17 N2 O2		
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.50	Report
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C00B	3.93	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	16	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	5	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O8 .	132.7	Degree

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PLAT432_ALERT_2_G Short Inter X...Y Contact C11 ..C35 . 3.20 Ang.
                                     x,-y,-1/2+z = 6_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 19 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 21 Note
      O014 N001 C004 H004 C006 H006 C007 H007
      C009 H009 C00J H00J C002 H002 C00A C00B
      C00C H00C C00I H00I C00K
PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data 4 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 26 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]= 0.07 Note
      2 0 0, 4 0 0,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
      4 0 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.2 Low
PLAT948_ALERT_5_G Externally Supplied Scattering Factors RES 4 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 11 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 11 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.648 Note
      Predicted wR2: Based on SigI**2 24.63 or SHELX Weight 58.76 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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- 4 **ALERT level A** = Most likely a serious problem - resolve or explain
 5 **ALERT level B** = A potentially serious problem, consider carefully
 17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 30 **ALERT level G** = General information/check it is not something unexpected
- 9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
 20 ALERT type 3 Indicator that the structure quality may be low
 9 ALERT type 4 Improvement, methodology, query or suggestion
 5 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 b - ellipsoid plot

