



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_1605_auto

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_1605_auto

Bond precision:	C-C = 0.0417 Å		Wavelength=0.02510
Cell:	a=8.1 (2)	b=9.52 (17)	c=45.1 (3)
	alpha=90	beta=91.39 (10)	gamma=90
Temperature:	97 K		
	Calculated	Reported	
Volume	3477 (108)	3470 (118)	
Space group	I 2/a	I 1 2/a 1	
Hall group	-I 2ya	-I 2ya	
Moiety formula	C22 H20 N2 O2 [+ solvent]	C22 H20 N2 O2	
Sum formula	C22 H20 N2 O2 [+ solvent]	C22 H19 N2 O2	
Mr	344.40	343.41	
Dx, g cm-3	1.320	1.315	
Z	8	8	
Mu (mm-1)	0.000	0.000	
F000	0.0	589.0	
F000'	1455.76		
h, k, lmax	8, 10, 47	8, 10, 47	
Nref	2192	1819	
Tmin, Tmax		0.157, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.157 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.830

Theta (max)= 0.765

R(reflections)= 0.2115(918)

wR2(reflections)=
0.6136(1819)

S = 1.232

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 = 0.5319

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 . 0.831 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) 0.61 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 0.21 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 0.10 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 26 Report
O00F O00N N00B N00J C002 C004 C00A C00C
C00I C00D C001 C005 C007 C006 C003 C00L
C008 C009 C00E C00G C00H C00K C00M C00O
C00P C00Q

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 0.04174 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= 0.532 368 Report
-2 0 4, -2 0 6, 0 0 6, -4 0 8, -2 0 8, 0 0 8,
-1 1 8, -2 1 9, -4 0 10, -2 0 10, 0 0 10, -1 1 10,
-2 1 11, -6 0 12, -4 0 12, -2 0 12, 0 0 12, -3 1 12,
-1 1 12, -4 1 13, -2 1 13, -1 2 13, -6 0 14, -4 0 14,
-2 0 14, 0 0 14, -3 1 14, -1 1 14, -2 2 14, -4 1 15,
(338 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 0.155

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	0.155	Report
PLAT148_ALERT_3_C	s.u. on the a - Axis is (Too) Large		0.200	Ang.
PLAT148_ALERT_3_C	s.u. on the b - Axis is (Too) Large		0.1700	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		C00G	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours		C00M	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours		O00F	Check
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C00O - C00P .		1.43	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H00E ..H00F .		1.99	Ang.
	x,y,z =	1_555		Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		25.083	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		7.156	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.736	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: C22 H19 N2 O2
 Atom count from _chemical_formula_moiety: C22 H20 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: C22 H19 N2 O2
 Atom count from the _atom_site data: C22 H20 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 C22 H19 N2 O2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	176.00	176.00	0.00
H	152.00	160.00	-8.00
N	16.00	16.00	0.00
O	16.00	16.00	0.00

RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.
 Radiation given as transmission electron microscope
 Radiation identified as electron

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	26	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
	H00B		
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please	Check
	Calc: C22 H20 N2 O2		
	Rep.: C22 H19 N2 O2		
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.40	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-10	Units
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C00E	7.23	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	5	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report

PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	9 A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	46 Note
	C002 C004 C00A H00A C00C H00C C00I H00I	
	C00D H00D C001 C005 C007 H007 C006 H006	
	C003 C00L H00L C008 H008 C009 N00B H00B	
	C00E H00E O00F C00G C00H H00H N00J C00K	
	C00M H00F H00G O00N C00O H00J H00K C00P	
	H00M H00N C00Q H00O H00P H00Q	
PLAT768_ALERT_4_G	RES Embedded Explicitly Supplied Scattering Data	4 Note
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]=	0.08 Note
	0 0 2, 0 0 4,	
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
	-2 0 6,	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.8 Low
PLAT948_ALERT_5_G	Externally Supplied Scattering Factors RES	4 Note
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1 Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	8.292 Note
	Predicted wR2: Based on SigI**2 7.40 or SHELX Weight 49.83	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 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
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 32 **ALERT level G** = General information/check it is not something unexpected
- 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 18 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
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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

