



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_1360

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_1360

Bond precision:	C-C = 0.0810 Å	Wavelength=0.02510	
Cell:	a=8.3 (4)	b=9.1 (5)	c=43.9 (8)
	alpha=90	beta=91.7 (2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3314 (250)	3345 (256)	
Space group	I 2/c	I 1 2/c 1	
Hall group	-I 2yc	-I 2yc	
Moiety formula	C20 H16 N2 O2 [+ solvent]	C20 H16 N2 O2	
Sum formula	C20 H16 N2 O2 [+ solvent]	C20 H15 N2 O2	
Mr	316.35	315.35	
Dx, g cm-3	1.270	1.253	
Z	8	8	
Mu (mm-1)	0.000	0.000	
F000	0.0	532.0	
F000'	1327.77		
h, k, lmax	8, 9, 43	8, 9, 43	
Nref	1680	1670	
Tmin, Tmax		0.118, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.118 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta (max)= 0.712

R(reflections)= 0.4178(534)

wR2(reflections)=
0.7916(1670)

S = 1.254

Npar= 72

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.

PLAT082_ALERT_2_A High R1 Value 0.42 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) 0.79 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 0.192

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 0.192 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 .. 32% 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.

PLAT149_ALERT_3_B s.u. on the beta Angle is Too Large 0.20 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 24 Report

O020	O27	N004	N009	C003	C005	C006	C012
C018	C013	C008	C010	C007	C011	C015	C017
C021	C019	C001	C002	C016	C014	C022	C029

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 0.08095 Ang.

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



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	0.5000 Ang.
PLAT148_ALERT_3_C s.u. on the	c	- Axis is (Too) Large	0.800 Ang.

PLAT160_ALERT_4_C	max(sig)/min(sig) ratio x,y,z > 3 for C017	14.93	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C003	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C006	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C011	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C015	Check
PLAT241_ALERT_2_C	High MainResAtom Ueq as Compared to Neighbours	C021	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	N004	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C012	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C010	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C001	Check
PLAT242_ALERT_2_C	Low MainResAtom Ueq as Compared to Neighbours	C014	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	45.450	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.434	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	22.070	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.377	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.141	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.111	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.079	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.045	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.788	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.126	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.453	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.019	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.408	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.004	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.496	29	Report
	-2 0 2, -4 0 4, -2 0 4, -6 0 6, -4 0 6, -2 0 6,		
	-8 0 8, -6 0 8, -4 0 8, -2 0 8, -8 0 10, -6 0 10,		
	-4 0 10, -2 0 10, -6 0 12, -4 0 12, -6 0 14, -4 0 14,		
	-6 0 16, -4 0 16, -6 0 18, -4 0 18, -6 0 20, -4 0 20,		
	-6 0 22, -6 0 24, -6 0 26, -6 0 28, -6 0 30,		
PLAT977_ALERT_2_C	Check Negative Difference Density on H017 .	-0.38	eA-3

● 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: C20 H15 N2 O2
 Atom count from _chemical_formula_moiety: C20 H16 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: C20 H15 N2 O2
 Atom count from the _atom_site data: C20 H16 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 C20 H15 N2 O2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	160.00	160.00	0.00
H	120.00	128.00	-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			16 Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms			24 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
H009				
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ			Please Check
	Calc: C20 H16 N2 O2			
	Rep.: C20 H15 N2 O2			
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large			0.50 Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...			-6 Units
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C011			7.88 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C001			5.18 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C002			8.29 Check
PLAT160_ALERT_4_G	max(sig)/min(sig) ratio x,y,z > 3 for C016			7.77 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			11 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records			8 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
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU 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
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature			293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature			293 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure			35 A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels			39 Note
	C003 H003 N004 C005 C006 H006 C012 C018			
	H018 C013 H013 C008 C010 H010 C007 N009			
	H009 C011 C015 C017 H017 O020 C021 H021			
	C019 H019 C001 C002 C016 H016 C014 H014			
	C022 H02A H02B H02C C029 H02D H02E			
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...			0.01 Ang.
	C029 -H02E 1_555 1_555	#		44 Check
PLAT768_ALERT_4_G	RES Embedded Explicitly Supplied Scattering Data			4 Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C007 --C017			2.48 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...			29.30 Deg.
	C015 -C007 -C017 1_555 1_555 7_555	#		28 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			65 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 ..			70.08% Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			2.5 Low
PLAT948_ALERT_5_G	Externally Supplied Scattering Factors RES			4 Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value			2.785 Note
	Predicted wR2: Based on SigI**2 28.42 or SHELX Weight 63.14			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
6 **ALERT level B** = A potentially serious problem, consider carefully
32 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
39 **ALERT level G** = General information/check it is not something unexpected
- 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

20 ALERT type 2 Indicator that the structure model may be wrong or deficient
27 ALERT type 3 Indicator that the structure quality may be low
18 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

