



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3d, 5p, 6p, 8a

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: 3d

Bond precision:	C-C = 0.0029 Å	Wavelength=1.54184	
Cell:	a=17.4943 (12) alpha=90	b=7.3922 (5) beta=103.709 (2)	c=12.5448 (8) gamma=90
Temperature:	108 K		
	Calculated	Reported	
Volume	1576.09 (18)	1576.09 (18)	
Space group	C 2	C 2	
Hall group	C 2y	C 2y	
Moiety formula	C20 H18 N2 O	C20 H18 N2 O	
Sum formula	C20 H18 N2 O	C20 H18 N2 O	
Mr	302.36	302.36	
Dx, g cm ⁻³	1.274	1.274	
Z	4	4	
Mu (mm ⁻¹)	0.624	0.624	
F000	640.0	640.0	
F000'	641.78		
h, k, lmax	21, 8, 15	21, 8, 15	
Nref	2920 [1583]	2821	
Tmin, Tmax	0.836, 0.905	0.777, 1.000	
Tmin'	0.819		

Correction method= # Reported T Limits: Tmin=0.777 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 1.78/0.97 Theta(max)= 68.742

R(reflections)= 0.0317(2779)

wR2(reflections)=
0.0771(2821)

S = 1.078

Npar= 210

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 C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report
12 0 0, 14 0 0, -14 0 1, -10 0 1, -2 0 1, 2 0 1,
14 6 1, -10 0 2, 0 0 2, 2 0 2, 6 8 3, 0 0 4,
9 7 4, 14 0 4, -10 0 14,

Alert level G

PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C4 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
0 0 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.110 Note
Predicted wR2: Based on SigI**2 2.48 or SHELX Weight 7.15
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
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Datablock: 5p

Bond precision: C-C = 0.0035 A

Wavelength=0.71073

Cell: a=7.5188(6) b=12.057(1) c=14.2757(12)
alpha=90 beta=95.497(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1288.20(18)	1288.20(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C15 H14 N2 O2	C15 H14 N2 O2
Sum formula	C15 H14 N2 O2	C15 H14 N2 O2
Mr	254.28	254.28
Dx, g cm ⁻³	1.311	1.311
Z	4	4
Mu (mm ⁻¹)	0.089	0.089
F000	536.0	536.0
F000'	536.23	
h, k, lmax	10, 16, 19	10, 16, 19
Nref	3208	3165
Tmin, Tmax	0.965, 0.980	0.536, 1.000
Tmin'	0.949	

Correction method= # Reported T Limits: Tmin=0.536 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 0.987 Theta(max)= 28.343

R(reflections)= 0.0887(2224) wR2(reflections)=
0.2908(3165)

S = 1.076 Npar= 174

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 C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.29	Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...	-1.158	Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600		26 Report
-1 3 3, 0 4 3, 0 10 8, -3 7 9, 1 10 9, -5 6 10,		
-2 8 10, -3 9 10, 1 9 10, -1 8 11, -4 9 11, -1 11 11,		
-4 0 12, -4 1 12, -4 2 12, -5 7 12, -3 7 12, -3 8 12,		
1 9 12, 2 9 12, -3 0 13, -3 3 13, -4 5 13, 0 9 13,		
-4 2 15, -2 0 16,		

● Alert level G

PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	17	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	4.4	Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	3.965	Note
Predicted wR2: Based on SigI**2 7.33 or SHELX Weight 27.03		
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	1	Info

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Datablock: 6p

Bond precision: C-C = 0.0019 A

Wavelength=0.71073

Cell: a=9.696(3) b=12.448(4) c=12.746(4)
alpha=84.369(7) beta=68.207(7) gamma=68.928(7)

Temperature: 100 K

	Calculated	Reported
Volume	1331.8(7)	1331.8(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C15 H14 N2 O2	C15 H14 N2 O2
Sum formula	C15 H14 N2 O2	C15 H14 N2 O2
Mr	254.28	254.28
Dx, g cm-3	1.268	1.268
Z	4	4
Mu (mm-1)	0.086	0.086
F000	536.0	536.0
F000'	536.23	
h, k, lmax	12, 16, 16	12, 16, 16
Nref	6586	6407
Tmin, Tmax	0.948, 0.984	0.845, 1.000
Tmin'	0.921	

Correction method= # Reported T Limits: Tmin=0.845 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 0.973

Theta(max)= 28.271

R(reflections)= 0.0472(5484)

wR2(reflections)=
0.1181(6407)

S = 1.079

Npar= 347

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 C**

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.088 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 39 Report
3 4 1, -5 0 7, 7 -7 8, 8 -5 8, 9 -4 8, 4 -9 9,
5 -8 9, 8 -5 9, 9 -3 9, 9 -2 9, 0-10 10, 2 -9 10,
3 -8 10, 5 -8 10, 6 -7 10, 7 -4 10, 8 -3 10, 9 -2 10,
9 -1 10, 1 -9 11, 3 -8 11, 4 -8 11, 0 -7 11, 5 -7 11,
7 -5 11, 7 -4 11, 9 -2 11, 0 -7 12, 3 -7 12, 4 -7 12,
(9 More Missing: see the .ckf listing file)

● **Alert level G**

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.96 mm
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.007 Degree
PLAT230_ALERT_2_G Hirshfeld Test Diff for C10 --C13 . 6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C110 --C113 . 5.8 s.u.
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C102 Check
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C105 Check
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SpGr) R Verify
PLAT793_ALERT_4_G Model has Chirality at C5 (Centro SpGr) R Verify
PLAT793_ALERT_4_G Model has Chirality at C102 (Centro SpGr) R Verify
PLAT793_ALERT_4_G Model has Chirality at C105 (Centro SpGr) R Verify
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL 2019/3 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 1.75 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 138 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
0 0 1, 6 -7 12, 7 -6 12, 6 -6 13, 7 -5 13,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.039 Note
Predicted wR2: Based on SigI**2 3.89 or SHELX Weight 10.95
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 11 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 3 Check

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Datablock: 8a

PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta (Min) [Deg]= 0 2 0,	2.25	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 0 2 0,	1	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value Predicted wR2: Based on SigI**2 4.64 or SHELX Weight 13.08	3.035	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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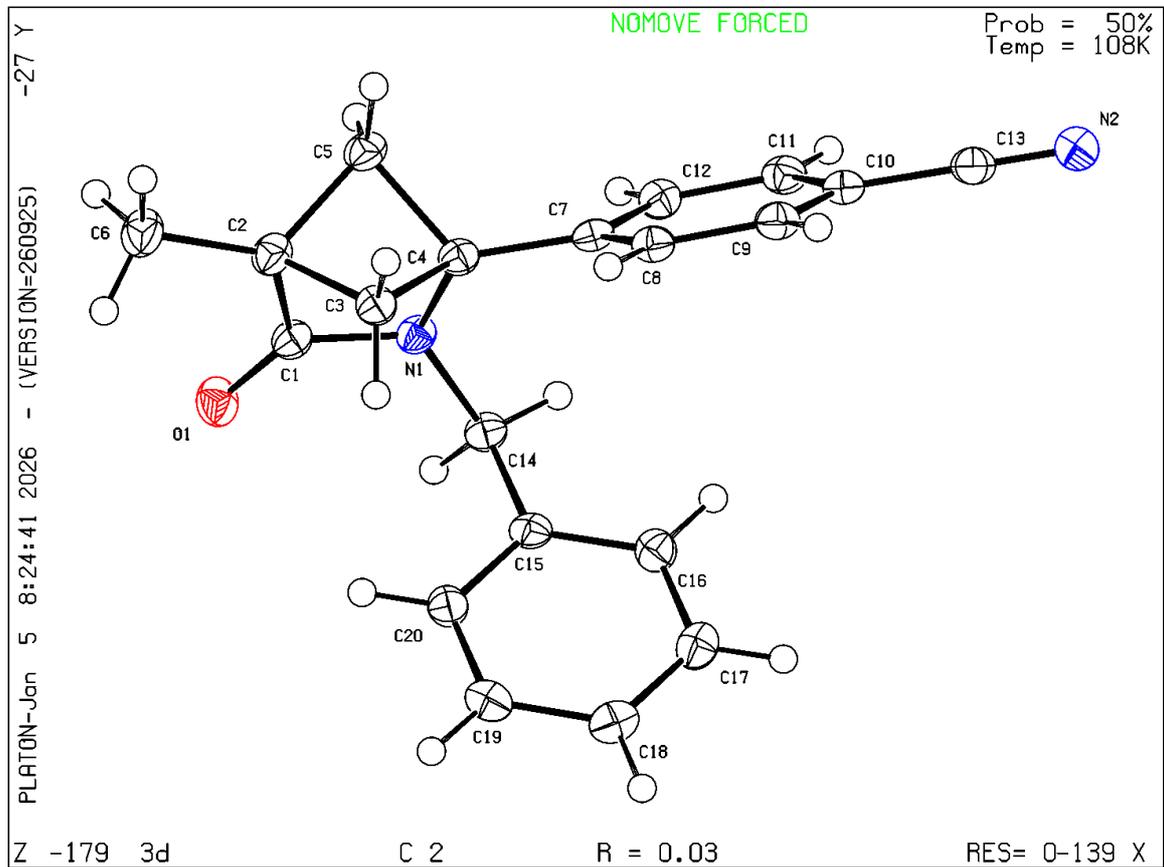
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found



Datablock 5p - ellipsoid plot

