

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: f

Bond precision: C-C = 0.0026 Å Wavelength=0.71073

Cell: a=16.0616(8) b=10.0135(6) c=22.6857(14)
alpha=90 beta=101.655(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	3573.4(4)	3573.4(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C18 H26 N3 O2	C18 H26 N3 O2
Sum formula	C18 H26 N3 O2	C18 H26 N3 O2
Mr	316.42	316.42
Dx, g cm ⁻³	1.176	1.176
Z	8	8
Mu (mm ⁻¹)	0.078	0.078
F000	1368.0	1368.0
F000'	1368.53	
h, k, lmax	21, 13, 30	21, 13, 30
Nref	4578	4578
Tmin, Tmax	0.985, 0.986	0.985, 0.986
Tmin'	0.985	

Correction method= # Reported T Limits: Tmin=0.985
Tmax=0.986 AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 28.580

R(reflections)= 0.0512(3132) wR2(reflections)= 0.1691(4578)

S = 0.969 Npar= 208

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**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.24	Report
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C4	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N3	Check
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	42	Ang3

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K) 293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	(K) 293 Check
PLAT793_ALERT_4_G	The Model has Chirality at C15 (Centro SPGR)	R Verify
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 0 ALERT type 3 Indicator that the structure quality may be low
- 2 ALERT type 4 Improvement, methodology, query or suggestion
- 1 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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

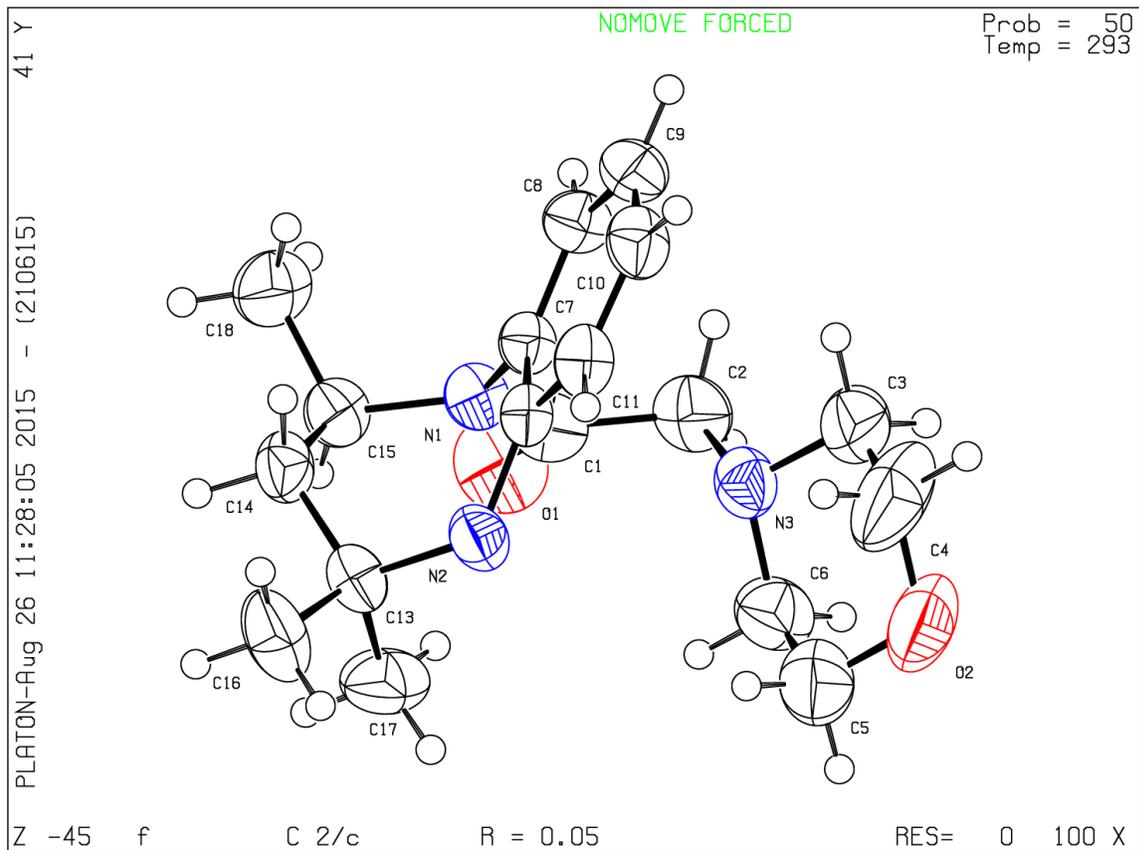
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock f - ellipsoid plot



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