
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**

PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 --C2 .	6.0 s.u.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N2 --H2 .	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.152 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.98Ang From N2 .	-0.52 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H2 .	-0.38 eA-3

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	76 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	5 Note
PLAT953_ALERT_1_G	Reported (CIF) and Actual (FCF) Hmax Differ by .	1 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	10 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
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- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 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.

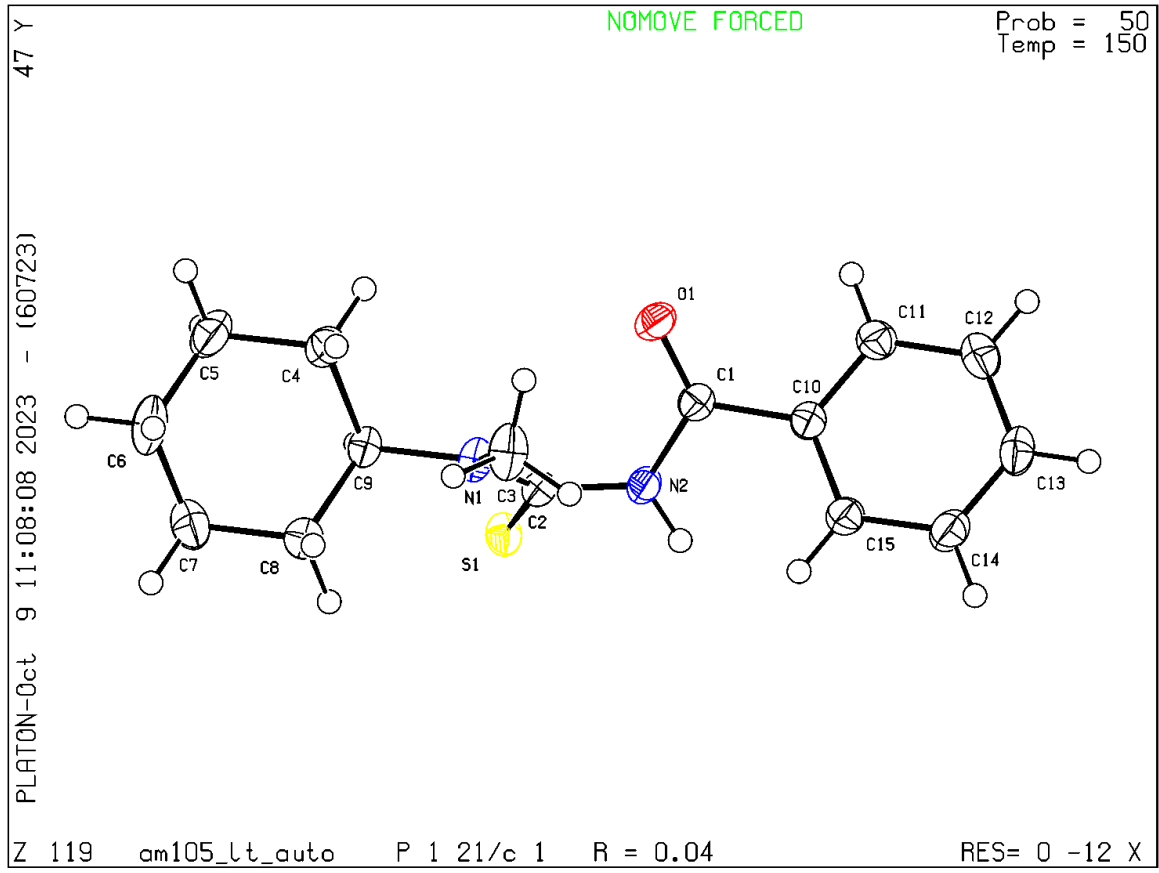
Publication of your CIF in IUCr journals

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* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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PLATON version of 06/07/2023; check.def file version of 30/06/2023



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PLAT230_ALERT_2_C	Hirshfeld Test Diff for	S1	--C2	.	5.2 s.u.
PLAT414_ALERT_2_C	Short Intra D-H..H-X	H2	..H11	.	1.97 Ang.
			x,y,z =	1_555	Check
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang	From N2	.	-0.41 eA-3

● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	698	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	13	Info

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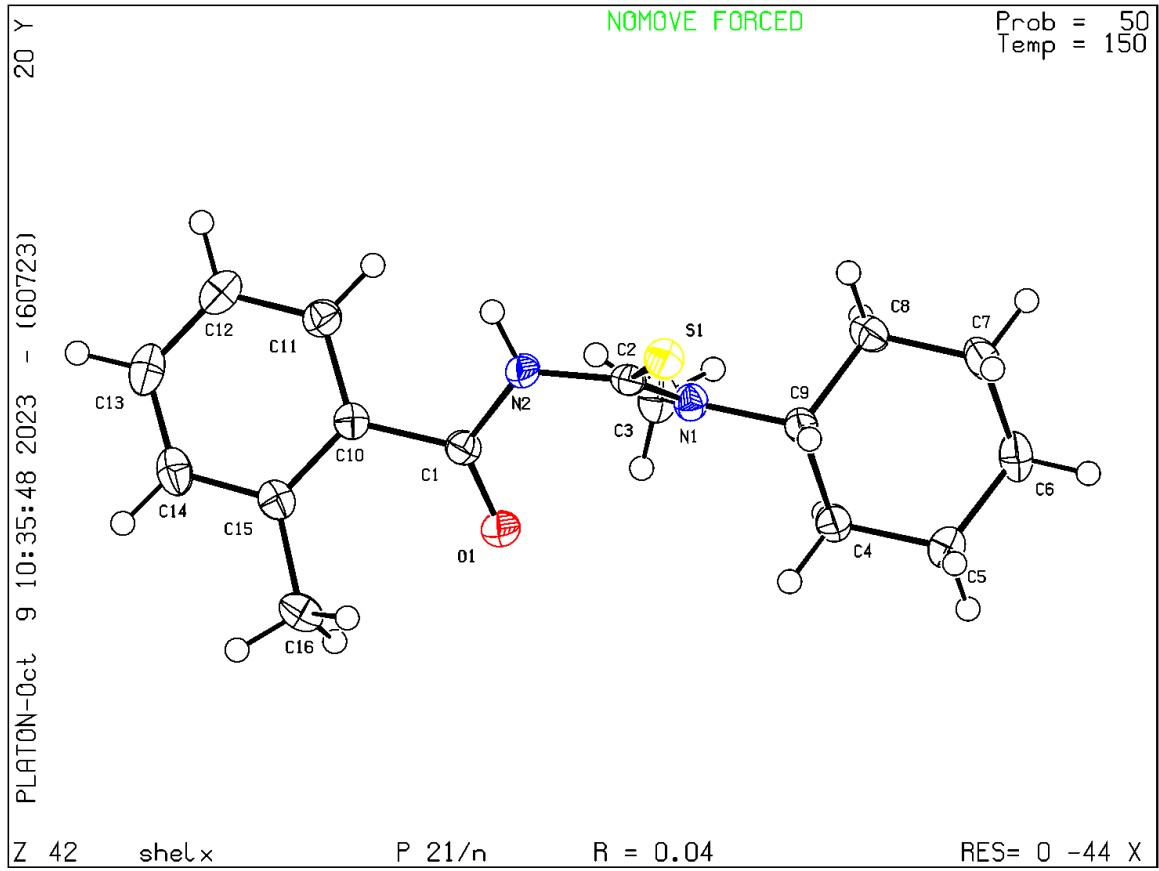
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PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	40 Report

● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1037 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.5 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	11 Info

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