

R(reflections)= 0.0670( 1373)	wR2(reflections)= 0.2083( 2544)
S = 1.006	Npar= 204

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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.

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### Alert level B

PLAT242_ALERT_2_B	Low	'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT242_ALERT_2_B	Low	'MainMol' Ueq as Compared to Neighbors of	C6A	Check
PLAT340_ALERT_3_B	Low	Bond Precision on C-C Bonds .....	0.01096	Ang.

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### Alert level C

STRVA01_ALERT_4_C		Flack parameter is too small		
		From the CIF: _refine_ls_abs_structure_Flack	-4.000	
		From the CIF: _refine_ls_abs_structure_Flack_su	1.000	
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please	Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		3.8	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range		3.7	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6A --C8A	.	0.16	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C15 H18 N2 O			
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	8	Report

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### Alert level G

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: C15 H18 N2 O1			
	Atom count from the _atom_site data: C15 H17.75 N2 O1			
CELLZ01_ALERT_1_G	Difference between formula and atom_site contents detected.			
CELLZ01_ALERT_1_G	WARNING: H atoms missing from atom site list. Is this intentional?			
	From the CIF: _cell_formula_units_Z	2		
	From the CIF: _chemical_formula_sum	C15 H18 N2 O		
	TEST: Compare cell contents of formula and atom_site data			
	atom	Z*formula	cif sites	diff
	C	30.00	30.00	0.00
	H	36.00	35.50	0.50
	N	4.00	4.00	0.00
	O	2.00	2.00	0.00
PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF .....	Please	Check
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High	.	1.000	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1AC	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8AC	Constrained at	0.5	Check

PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond C6 - C7 .	1.51 Ang.
PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond C6A - C8A .	1.50 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9 Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	12 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C15 H18 N2 O	
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	4 Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17 Note
PLAT915_ALERT_3_G	No Flack x Check Done: Low Friedel Pair Coverage	33 %
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	3.50 Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
10 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
21 ALERT type 4 Improvement, methodology, query or suggestion  
0 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. 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.

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

Datablock exp\_215 - ellipsoid plot

