

R(reflections)= 0.0310(7050)	wR2(reflections)= 0.0794(7834)
S = 1.039	Npar= 487

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

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.14	Do !
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	N10	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C24	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C32	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	U1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Rh1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Rh2	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.01058	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C28 - C29	1.43	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C32 - C33	1.43	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	9	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on	H20B	-0.32	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H32A	-0.36	eA-3

 Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	13.72 Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	5	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	U1 --N4	8.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	U1 --N7	9.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Rh1 --N4	5.5 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for U1	(IV)	3.88 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	96	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	6 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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
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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.

