

R(reflections)= 0.0776(3308)	wR2(reflections)= 0.2077(8887)
S = 0.935	Npar= 667

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 B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 37% Check

Author Response: This is caused by the weak diffraction of the sample.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.147

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.147	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C49 --C52 .	5.5	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C53 --C61 .	5.5	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9 --C10 .	0.17	Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00653	Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check



Alert level G

PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.9 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0 Degree

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected
- 1 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
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.

