

R(reflections)= 0.0171(5853)	wR2(reflections)= 0.0307(6102)
S = 1.128	Npar= 693

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

PLAT089_ALERT_3_B Poor Data / Parameter Ratio (Zmax < 18) 5.12 Note

Author Response: Attempt was made using NoSpherA2 to perform HAR refinement as far as possible with well-diffracting crystal within a high (but not ultra) resolution sphere.



Alert level C

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.2 Ratio
PLAT245_ALERT_2_C U(iso) H1 Smaller than U(eq) C1 by 0.012 Ang**2
PLAT245_ALERT_2_C U(iso) H1B Smaller than U(eq) C1B by 0.011 Ang**2



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 38 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 23 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 32% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O4 . 109.7 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note
PLAT791_ALERT_4_G Model has Chirality at C1 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C2 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C3 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) R Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 484 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 141 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 18 Info
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used Please Note

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

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
5 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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.