

```
R(reflections)= 0.0687( 1338)      wR2(reflections)=
S = 1.038                        0.1862( 2426)
Npar= 185
```

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

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: `_refine_ls_abs_structure_Flack` 1.000
From the CIF: `_refine_ls_abs_structure_Flack_su` 3.000
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 7.39 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00883 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.237 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 1.00 Check

● Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: `_cell_formula_units_Z` 4
From the CIF: `_chemical_formula_sum` C17 H11 F4 N O0
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	68.00	68.00	0.00
H	44.00	44.00	0.00
F	16.00	16.00	0.00
N	4.00	4.00	0.00
O	4.00	0.00	4.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 17 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 3.000 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0010 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 42 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). 4 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.50 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.6 Low
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by . 1 Units
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected

- 4 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
8 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
-

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.

