

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

| | | | |
|-----------------|----------------|--------------------|--------------|
| Bond precision: | C-C = 0.0042 A | Wavelength=1.54187 | |
| Cell: | a=10.1431(5) | b=37.2421(15) | c=10.4416(5) |
| | alpha=90 | beta=105.318(2) | gamma=90 |
| Temperature: | 293 K | | |

```
Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.833
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0424( 15512)      wR2(reflections)=
S = 1.015                          0.0569( 15714)
Npar= 525
```

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 A

DIFMN02_ALERT_2_A The minimum difference density is $< -0.1 \times Z_{MAX} \times 2.00$
_refine_diff_density_min given = -8.850
Test value = -3.400

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 4.69 eA-3

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT098_ALERT_2_A Large Reported Min. (Negative) Residual Density -8.85 eA-3

Author Response: Although the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT703_ALERT_1_A Torsion Calc -170.1(2), Rep -169.4(3), Dev.. 3.50 Sigma
N(1)-S(1)-C(1)-C(31 1_555 1_555 1_555 1_555 # 10 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc -44.7(2), Rep -43.7(3), Dev.. 5.00 Sigma
C(50-N(2)-C(17-C(48 1_555 1_555 1_555 1_555 # 45 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc -174.02(19), Rep -175.0(3), Dev.. 5.16 Sigma
C(50-N(2)-C(35-C(29 1_555 1_555 1_555 1_555 # 47 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc 56.2(2), Rep 55.4(4), Dev.. 4.00 Sigma
 C(50-N(2)-C(35-C(44 1_555 1_555 1_555 1_555 # 48 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc 55.5(2), Rep 54.6(5), Dev.. 4.50 Sigma
 C(45-N(3)-C(28-C(30 1_555 1_555 1_555 1_555 # 50 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc -176.33(18), Rep -177.1(3), Dev.. 4.28 Sigma
 C(45-N(3)-C(28-C(42 1_555 1_555 1_555 1_555 # 51 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc -24.9(3), Rep -23.9(5), Dev.. 3.33 Sigma
 N(3)-C(45-C(51-C(52 1_555 1_555 1_555 1_555 # 136 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_A Torsion Calc -0.8(3), Rep -2.1(5), Dev.. 4.33 Sigma
 C(45-C(51-C(52-C(46 1_555 1_555 1_555 1_555 # 140 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.



Alert level B

REFLT02_ALERT_1_B The number of reflections greater than the sigma threshold cannot exceed the number of symmetry-independent reflections

Number of symmetry-independent reflections = 7156

Number of reflections greater than sigma threshold = 15512

PLAT230_ALERT_2_B Hirshfeld Test Diff for S2 --O9 . 7.9 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for S2 --O12 . 7.9 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for O6 --C37 . 7.7 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for N3 --C46 . 7.3 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O8 . 10.5 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --N1 . 8.3 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for O2 --C41 . 8.0 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for O2 --C54 . 7.5 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for N2 --C17 . 7.7 s.u.
 PLAT230_ALERT_2_B Hirshfeld Test Diff for C1 --C31 . 7.3 s.u.
 PLAT703_ALERT_1_B Torsion Calc -176.4(3), Rep -175.7(6), Dev.. 2.33 Sigma
 C(47-O(3)-C(36-C(25 1_555 1_555 1_555 1_555 # 29 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc -164.6(2), Rep -165.1(4), Dev.. 2.50 Sigma
C(28-N(3)-C(46-C(52 1_555 1_555 1_555 1_555 # 52 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc 172.1(2), Rep 171.6(4), Dev.. 2.50 Sigma
C(46-N(3)-C(28-C(30 1_555 1_555 1_555 1_555 # 53 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc 174.6(2), Rep 175.2(4), Dev.. 3.00 Sigma
S(1)-C(1)-C(29-C(40 1_555 1_555 1_555 1_555 # 62 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc 179.8(2), Rep -179.7(4), Dev.. 2.50 Sigma
N(1)-C(2)-C(39-C(26 1_555 1_555 1_555 1_555 # 67 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc -132.7(2), Rep -133.2(4), Dev.. 2.50 Sigma
C(40-C(29-C(35-C(44 1_555 1_555 1_555 1_555 # 113 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc 26.4(3), Rep 27.3(5), Dev.. 3.00 Sigma
N(3)-C(46-C(52-C(51 1_555 1_555 1_555 1_555 # 137 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_B Torsion Calc -29.2(2), Rep -28.7(4), Dev.. 2.50 Sigma
N(2)-C(50-C(53-C(48 1_555 1_555 1_555 1_555 # 139 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.960 Why?

PLAT230_ALERT_2_C Hirshfeld Test Diff for O6 --C47 . 7.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C1 --C29 . 5.7 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C26 --C41 . 7.0 s.u.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C54 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C49 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00418 Ang.

PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS <= 32 Ang**3

PLAT703_ALERT_1_C Torsion Calc -101.5(3), Rep -101.9(5), Dev.. 1.33 Sigma
O(1)-S(1)-C(1)-C(29) 1_555 1_555 1_555 1_555 # 3 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 74.0(2), Rep 74.4(4), Dev.. 2.00 Sigma
O(1)-S(1)-C(1)-C(31) 1_555 1_555 1_555 1_555 # 4 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 131.0(3), Rep 130.5(4), Dev.. 1.67 Sigma
O(8)-S(1)-C(1)-C(29) 1_555 1_555 1_555 1_555 # 7 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -53.5(2), Rep -53.2(4), Dev.. 1.50 Sigma
O(8)-S(1)-C(1)-C(31) 1_555 1_555 1_555 1_555 # 8 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -6.0(2), Rep -6.3(3), Dev.. 1.50 Sigma
O(12)-S(2)-N(4)-C(21) 1_555 1_555 1_555 1_555 # 17 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -177.03(17), Rep -176.7(2), Dev.. 1.94 Sigma
N(4)-S(2)-C(32)-C(23) 1_555 1_555 1_555 1_555 # 21 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 8.5(3), Rep 9.0(6), Dev.. 1.67 Sigma
C(37-O(6)-C(47-O(3) 1_555 1_555 1_555 1_555 # 31 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -5.8(4), Rep -6.4(6), Dev.. 1.50 Sigma
C(47-O(6)-C(37-C(36) 1_555 1_555 1_555 1_555 # 33 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 80.9(3), Rep 80.5(5), Dev.. 1.33 Sigma
C(27-N(1)-C(2)-C(39) 1_555 1_555 1_555 1_555 # 39 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 163.97(19), Rep 164.3(3), Dev.. 1.74 Sigma
C(28-N(3)-C(45-C(51) 1_555 1_555 1_555 1_555 # 49 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -102.8(3), Rep -103.4(4), Dev.. 2.00 Sigma
S(2)-N(4)-C(24-C(19) 1_555 1_555 1_555 1_555 # 57 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 82.7(3), Rep 82.2(5), Dev.. 1.67 Sigma
C(21-N(4)-C(24-C(19) 1_555 1_555 1_555 1_555 # 59 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -8.8(4), Rep -8.1(8), Dev.. 1.75 Sigma
S(1)-C(1)-C(29-C(35) 1_555 1_555 1_555 1_555 # 61 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 0.3(4), Rep 0.8(8), Dev.. 1.25 Sigma
C(29-C(1)-C(31-C(33 1_555 1_555 1_555 1_555 # 64 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 4.1(4), Rep 3.6(6), Dev.. 1.25 Sigma
N(1)-C(2)-C(44-C(35 1_555 1_555 1_555 1_555 # 69 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -176.1(2), Rep -176.4(4), Dev.. 1.50 Sigma
C(39-C(2)-C(44-C(35 1_555 1_555 1_555 1_555 # 71 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 176.6(2), Rep 177.0(4), Dev.. 2.00 Sigma
C(41-C(3)-C(44-C(35 1_555 1_555 1_555 1_555 # 74 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -179.2(3), Rep -178.8(4), Dev.. 1.33 Sigma
C(44-C(3)-C(41-O(2) 1_555 1_555 1_555 1_555 # 75 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 25.7(2), Rep 25.4(3), Dev.. 1.50 Sigma
N(2)-C(17-C(48-C(53 1_555 1_555 1_555 1_555 # 77 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.8(5), Rep 0.0(8), Dev.. 1.60 Sigma
C(24-C(19-C(37-C(36 1_555 1_555 1_555 1_555 # 79 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.4(4), Rep -0.9(7), Dev.. 1.25 Sigma
C(37-C(19-C(24-C(30 1_555 1_555 1_555 1_555 # 81 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 178.16(19), Rep 177.8(3), Dev.. 1.89 Sigma
C(32-C(23-C(49-CL(1 1_555 1_555 1_555 1_555 # 82 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.4(4), Rep 0.2(5), Dev.. 1.50 Sigma
C(32-C(23-C(49-C(38 1_555 1_555 1_555 1_555 # 83 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -176.48(19), Rep -176.8(3), Dev.. 1.68 Sigma
C(49-C(23-C(32-S(2) 1_555 1_555 1_555 1_555 # 84 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 2.5(4), Rep 2.0(7), Dev.. 1.25 Sigma
N(4)-C(24-C(30-C(28 1_555 1_555 1_555 1_555 # 87 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 0.7(4), Rep 1.2(7), Dev.. 1.25 Sigma
C(19-C(24-C(30-C(25 1_555 1_555 1_555 1_555 # 88 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -1.1(5), Rep -0.3(7), Dev.. 1.60 Sigma
C(30-C(25-C(36-C(37 1_555 1_555 1_555 1_555 # 91 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 0.0(4), Rep -0.6(7), Dev.. 1.50 Sigma
C(36-C(25-C(30-C(24 1_555 1_555 1_555 1_555 # 92 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.4(4), Rep -1.0(6), Dev.. 1.50 Sigma
O(7)-C(26-C(41-O(2) 1_555 1_555 1_555 1_555 # 95 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 1.7(5), Rep 2.6(9), Dev.. 1.80 Sigma
C(39-C(26-C(41-C(3) 1_555 1_555 1_555 1_555 # 98 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -1.2(4), Rep -2.0(8), Dev.. 2.00 Sigma
C(41-C(26-C(39-C(2) 1_555 1_555 1_555 1_555 # 99 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 50.7(4), Rep 50.1(7), Dev.. 1.50 Sigma
C(1)-C(29-C(35-C(44 1_555 1_555 1_555 1_555 # 109 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.8(5), Rep -1.4(8), Dev.. 1.20 Sigma
C(1)-C(31-C(33-C(43 1_555 1_555 1_555 1_555 # 115 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 176.38(19), Rep 176.6(3), Dev.. 1.16 Sigma
S(2)-C(32-C(42-C(34 1_555 1_555 1_555 1_555 # 117 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 179.4(2), Rep 179.1(3), Dev.. 1.50 Sigma
C(38-C(34-C(42-C(28 1_555 1_555 1_555 1_555 # 122 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -0.4(4), Rep 0.3(6), Dev.. 1.75 Sigma
C(42-C(34-C(38-C(49 1_555 1_555 1_555 1_555 # 124 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc -67.3(3), Rep -66.7(5), Dev.. 2.00 Sigma
C(29-C(35-C(44-C(2) 1_555 1_555 1_555 1_555 # 127 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 1.1(4), Rep 1.7(7), Dev.. 1.50 Sigma
O(3)-C(36-C(37-O(6) 1_555 1_555 1_555 1_555 # 129 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 1.5(6), Rep 0.6(9), Dev.. 1.50 Sigma
C(25-C(36-C(37-C(19 1_555 1_555 1_555 1_555 # 132 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT703_ALERT_1_C Torsion Calc 1.1(4), Rep 0.3(6), Dev.. 2.00 Sigma
C(34-C(38-C(49-C(23 1_555 1_555 1_555 1_555 # 134 Check

Author Response: The structure is affected by some strain. Crystal imperfections can not be excluded either.

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C19 H19 Cl N2 O4 S



Alert level G

| | |
|--|--------------|
| PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF | Please Do ! |
| PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/a | P21/c Note |
| PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) | 293 Check |
| PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) | 293 Check |
| PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O3 . | 104.6 Degree |
| PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O6 . | 104.5 Degree |
| PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 . | 103.5 Degree |
| PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O7 . | 105.2 Degree |
| PLAT793_ALERT_4_G Model has Chirality at C28 (Centro SpGr) | R Verify |
| PLAT793_ALERT_4_G Model has Chirality at C35 (Centro SpGr) | S Verify |
| PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found | Please Check |
| PLAT882_ALERT_1_G No Datum for _diffn_reflms_av_unetI/netI | Please Do ! |
| PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. | Please Do ! |

11 **ALERT level A** = Most likely a serious problem - resolve or explain

19 **ALERT level B** = A potentially serious problem, consider carefully

51 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 13 **ALERT level G** = General information/check it is not something unexpected

63 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 23 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 4 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_REFLT02__143750_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143750_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143750_1
```

```

;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT230__143750_1
;
PROBLEM: Hirshfeld Test Diff for      S2      --O9      .      7.9 s.u.
RESPONSE: ...
;
_vrf_PLAT029__143750_1
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.960 Why?
RESPONSE: ...
;
_vrf_PLAT241__143750_1
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      C54 Check
RESPONSE: ...
;
_vrf_PLAT242__143750_1
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of      C49 Check
RESPONSE: ...
;
_vrf_PLAT340__143750_1
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00418 Ang.
RESPONSE: ...
;
_vrf_PLAT601__143750_1
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS      <=      32 Ang**3
RESPONSE: ...
;
_vrf_PLAT790__143750_1
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd.  #      1 Note
RESPONSE: ...
;
# end Validation Reply Form

```

PLATON version of 04/06/2025; check.def file version of 30/05/2025

