

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 = 0.0029 A	Wavelength=1.54187	
Cell:	a=8.8017 (4)	b=15.2880 (6)	c=12.7533 (5)
	alpha=90	beta=97.430 (2)	gamma=90
Temperature:	293 K		

```
Correction method= # Reported T Limits: Tmin=0.353 Tmax=0.638
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0427( 11055)      wR2(reflections)=
S = 1.162                          0.0642( 11129)
Npar= 267
```

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

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 4.89 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.

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00

_refine_diff_density_min given = -3.400

Test value = -1.700

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 = 3204

Number of reflections greater than sigma threshold = 11055

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -3.40 eA-3

PLAT213_ALERT_2_B Atom C22 has ADP max/min Ratio 4.6 prolat

PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O1 . 8.8 s.u.

PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --N1 . 10.5 s.u.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C22 Check

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O5 Check

PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C22 - C25 . 1.32 Ang.

PLAT703_ALERT_1_B Torsion Calc -50.01(14), Rep -50.40(19), Dev.. 2.79 Sigma

O(7)-S(1)-C(15-C(9) 1_555 1_555 1_555 1_555 # 7 Check

PLAT703_ALERT_1_B Torsion Calc 55.83(15), Rep 56.2(2), Dev.. 2.47 Sigma

C(24-S(3)-C(14-C(19) 1_555 1_555 1_555 1_555 # 15 Check

PLAT703_ALERT_1_B Torsion Calc 85.4(2), Rep 86.0(3), Dev.. 3.00 Sigma

C(12-N(1)-C(23-C(24) 1_555 1_555 1_555 1_555 # 25 Check

PLAT703_ALERT_1_B Torsion Calc 100.4(2), Rep 99.9(2), Dev.. 2.50 Sigma

C(23-N(1)-C(12-C(11) 1_555 1_555 1_555 1_555 # 26 Check

PLAT703_ALERT_1_B Torsion Calc 176.68(17), Rep 177.1(2), Dev.. 2.47 Sigma

C(13-C(10-C(16-C(14) 1_555 1_555 1_555 1_555 # 33 Check

PLAT703_ALERT_1_B Torsion Calc -179.45(16), Rep -179.8(2), Dev.. 2.19 Sigma

C(12-C(11-C(20-O(4) 1_555 1_555 1_555 1_555 # 36 Check

PLAT703_ALERT_1_B Torsion Calc 5.1(3), Rep 4.4(3), Dev.. 2.33 Sigma

N(1)-C(12-C(16-C(14) 1_555 1_555 1_555 1_555 # 41 Check

PLAT703_ALERT_1_B Torsion Calc -174.66(17), Rep -175.1(2), Dev.. 2.59 Sigma

C(11-C(12-C(16-C(14) 1_555 1_555 1_555 1_555 # 43 Check

PLAT703_ALERT_1_B Torsion Calc 66.3(2), Rep 66.9(2), Dev.. 3.00 Sigma

S(3)-C(14-C(16-C(12) 1_555 1_555 1_555 1_555 # 49 Check

PLAT703_ALERT_1_B Torsion Calc 118.49(19), Rep 118.1(2), Dev.. 2.05 Sigma

C(19-C(14-C(16-C(10) 1_555 1_555 1_555 1_555 # 54 Check

PLAT703_ALERT_1_B Torsion Calc -65.3(2), Rep -64.8(3), Dev.. 2.50 Sigma

C(19-C(14-C(16-C(12) 1_555 1_555 1_555 1_555 # 55 Check

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 _diffn_measured_fraction_theta_full value Low . 0.962 Why?

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H1 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H2 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H3 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H4 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H5 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H6 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H7 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H8 Note

PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged H9 Note

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.0 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for C12 --C18 . 5.8 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for S3 --C14 . 5.6 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C17 --C21 . 5.5 s.u.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check

PLAT245_ALERT_2_C U(iso) H4 Smaller than U(eq) C11 by 0.021 Ang**2

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C14 - H10 . 1.14 Ang.

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C23 - H8 . 1.11 Ang.

PLAT410_ALERT_2_C Short Intra H...H Contact H11 ..H14 . 1.91 Ang.

PLAT410_ALERT_2_C Short Intra H...H Contact H12 ..H13 . 1.91 Ang.

PLAT410_ALERT_2_C Short Intra H...H Contact H12 ..H13 . 1.91 Ang.

PLAT703_ALERT_1_C Torsion Calc -161.66(14), Rep -161.48(19), Dev.. 1.29 Sigma

O(1)-S(1)-N(1)-C(23 1_555 1_555 1_555 1_555 # 2 Check

PLAT703_ALERT_1_C Torsion Calc -103.18(15), Rep -102.9(2), Dev.. 1.87 Sigma

O(1)-S(1)-C(15-C(19 1_555 1_555 1_555 1_555 # 4 Check

PLAT703_ALERT_1_C Torsion Calc 174.83(11), Rep 174.61(15), Dev.. 2.00 Sigma

O(7)-S(1)-N(1)-C(12 1_555 1_555 1_555 1_555 # 5 Check

PLAT703_ALERT_1_C Torsion Calc 13.04(17), Rep 13.3(2), Dev.. 1.53 Sigma

N(1)-S(1)-C(15-C(19 1_555 1_555 1_555 1_555 # 10 Check

PLAT703_ALERT_1_C Torsion Calc -70.53(13), Rep -70.67(18), Dev.. 1.08 Sigma

C(15-S(1)-N(1)-C(12 1_555 1_555 1_555 1_555 # 11 Check

PLAT703_ALERT_1_C Torsion Calc -12.1(3), Rep -12.5(4), Dev.. 1.33 Sigma

C(20-O(4)-C(25-C(22 1_555 1_555 1_555 1_555 # 16 Check

PLAT703_ALERT_1_C Torsion Calc -179.58(16), Rep -179.4(2), Dev.. 1.13 Sigma

C(25-O(4)-C(20-C(11 1_555 1_555 1_555 1_555 # 17 Check

PLAT703_ALERT_1_C Torsion Calc 74.32(19), Rep 74.6(2), Dev.. 1.47 Sigma

S(1)-N(1)-C(12-C(16 1_555 1_555 1_555 1_555 # 23 Check

PLAT703_ALERT_1_C Torsion Calc -79.3(2), Rep -79.6(3), Dev.. 1.50 Sigma

C(23-N(1)-C(12-C(16 1_555 1_555 1_555 1_555 # 27 Check

PLAT703_ALERT_1_C Torsion Calc -179.13(14), Rep -178.91(18), Dev.. 1.57 Sigma

C(15-C(9)-C(18-CL(2 1_555 1_555 1_555 1_555 # 28 Check

PLAT703_ALERT_1_C Torsion Calc -0.9(3), Rep -0.4(3), Dev.. 1.67 Sigma

C(15-C(9)-C(18-C(21 1_555 1_555 1_555 1_555 # 29 Check

PLAT703_ALERT_1_C Torsion Calc 1.0(3), Rep 0.5(3), Dev.. 1.67 Sigma

C(18-C(9)-C(15-C(19 1_555 1_555 1_555 1_555 # 31 Check

PLAT703_ALERT_1_C Torsion Calc 0.4(3), Rep -0.1(3), Dev.. 1.67 Sigma

C(13-C(10-C(16-C(12 1_555 1_555 1_555 1_555 # 32 Check

PLAT703_ALERT_1_C Torsion Calc 177.08(16), Rep 177.3(2), Dev.. 1.38 Sigma

C(16-C(10-C(13-O(5) 1_555 1_555 1_555 1_555 # 34 Check

PLAT703_ALERT_1_C Torsion Calc -2.3(3), Rep -1.9(4), Dev.. 1.33 Sigma

C(16-C(10-C(13-C(20 1_555 1_555 1_555 1_555 # 35 Check

PLAT703_ALERT_1_C Torsion Calc -178.68(16), Rep	-178.4(2), Dev..	1.75 Sigma
N(1)-C(12-C(16-C(10	1_555 1_555 1_555 1_555	# 40 Check
PLAT703_ALERT_1_C Torsion Calc	1.6(3), Rep	2.0(4), Dev.. 1.33 Sigma
C(11-C(12-C(16-C(10	1_555 1_555 1_555 1_555	# 42 Check
PLAT703_ALERT_1_C Torsion Calc	2.0(3), Rep	2.4(4), Dev.. 1.33 Sigma
O(5)-C(13-C(20-O(4)	1_555 1_555 1_555 1_555	# 44 Check
PLAT703_ALERT_1_C Torsion Calc -178.65(16), Rep	-178.4(2), Dev..	1.56 Sigma
C(10-C(13-C(20-O(4)	1_555 1_555 1_555 1_555	# 46 Check
PLAT703_ALERT_1_C Torsion Calc -109.95(16), Rep	-110.2(2), Dev..	1.56 Sigma
S(3)-C(14-C(16-C(10	1_555 1_555 1_555 1_555	# 48 Check
PLAT703_ALERT_1_C Torsion Calc -178.52(13), Rep	-178.74(18), Dev..	1.69 Sigma
S(1)-C(15-C(19-C(17	1_555 1_555 1_555 1_555	# 57 Check
PLAT703_ALERT_1_C Torsion Calc 178.65(16), Rep	178.9(2), Dev..	1.56 Sigma
C(9)-C(15-C(19-C(14	1_555 1_555 1_555 1_555	# 58 Check

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 _diffrn_ambient_temperature (K)	293 Check
PLAT793_ALERT_4_G Model has Chirality at C14 (Centro SpGr)	S Verify
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflms_av_unetI/netI	Please Do !
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..	Please Do !

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 20 **ALERT level B** = A potentially serious problem, consider carefully
 - 45 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 8 **ALERT level G** = General information/check it is not something unexpected
-
- 40 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 4 ALERT type 3 Indicator that the structure quality may be low
 - 11 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_DIFMN02__143527_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*1.00
RESPONSE: ...
;
_vrf_REFLT02__143527_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143527_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143527_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT098__143527_1
```

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;
PROBLEM: Large Reported Min. (Negative) Residual Density -3.40 eA-3
RESPONSE: ...
;
_vrf_PLAT213__143527_1
;
PROBLEM: Atom C22 has ADP max/min Ratio ..... 4.6 prolat
RESPONSE: ...
;
_vrf_PLAT230__143527_1
;
PROBLEM: Hirshfeld Test Diff for S1 --O1 . 8.8 s.u.
RESPONSE: ...
;
_vrf_PLAT241__143527_1
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C22 Check
RESPONSE: ...
;
_vrf_PLAT242__143527_1
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of O5 Check
RESPONSE: ...
;
_vrf_PLAT360__143527_1
;
PROBLEM: Short C(sp3)-C(sp3) Bond C22 - C25 . 1.32 Ang.
RESPONSE: ...
;
_vrf_PLAT703__143527_1
;
PROBLEM: Torsion Calc -50.01(14), Rep -50.40(19), Dev.. 2.79 Sigma
RESPONSE: ...
;
_vrf_PLAT029__143527_1
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.962 Why?
RESPONSE: ...
;
_vrf_PLAT166__143527_1
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged .... H1 Note
RESPONSE: ...
;
_vrf_PLAT220__143527_1
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.0 Ratio
RESPONSE: ...
;
_vrf_PLAT222__143527_1
;
PROBLEM: NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
RESPONSE: ...
;
_vrf_PLAT245__143527_1
;
PROBLEM: U(iso) H4 Smaller than U(eq) C11 by 0.021 Ang**2

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*i**i*

RESPONSE: . . .

*i**i*

RESPONSE: . . .

i

Datablock_143527_1 - ellipsoid plot

