

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=11.2127 (6)	b=8.6727 (4)	c=18.8928 (9)
	alpha=90	beta=90.6559 (19)	gamma=90
Temperature:	293 K		

```
Correction method= # Reported T Limits: Tmin=0.625 Tmax=0.818
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0615( 11006)      wR2(reflections)=
S = 1.128                          0.0781( 11101)
Npar= 273
```

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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.

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### Alert level A

PLAT097\_ALERT\_2\_A Large Reported Max. (Positive) Residual Density 4.20 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.**

PLAT213\_ALERT\_2\_A Atom C23 has ADP max/min Ratio ..... 7.4 prolat

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

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### Alert level B

DIFMN02\_ALERT\_2\_B The minimum difference density is < -0.1\*ZMAX\*1.00

\_refine\_diff\_density\_min given = -2.550

Test value = -1.600

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 = 3536

Number of reflections greater than sigma threshold = 11006

PLAT098\_ALERT\_2\_B Large Reported Min. (Negative) Residual Density -2.55 eA-3

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for S1 --O2 . 10.2 s.u.

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for N1 --N2 . 13.3 s.u.

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C15 --C17 . 8.3 s.u.

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C19 --C23 . 36.5 s.u.

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C23 --C24 . 43.2 s.u.

PLAT245\_ALERT\_2\_B U(iso) H2 Smaller than U(eq) C17 by 0.064 Ang\*\*2

PLAT245\_ALERT\_2\_B U(iso) H4 Smaller than U(eq) N1 by 0.087 Ang\*\*2

PLAT360\_ALERT\_2\_B Short C(sp3)-C(sp3) Bond C19 - C25 . 1.30 Ang.

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### 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.

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	3.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	9.9	Ratio
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	S1	--O3	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	S1	--C8	.	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	N2	--C23	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	N4	--N5	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	N4	--C22	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	C1	--C10	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	C1	--C15	.	6.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	C17	--C20	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	C18	--C20	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld	Test	Diff for	C19	--C25	.	6.8 s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of		N1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of		N2	Check
PLAT245_ALERT_2_C	U(iso)	H1	Smaller than U(eq)	C15	by	0.019	Ang**2
PLAT245_ALERT_2_C	U(iso)	H8	Smaller than U(eq)	C11	by	0.014	Ang**2
PLAT245_ALERT_2_C	U(iso)	H9	Smaller than U(eq)	C12	by	0.031	Ang**2
PLAT340_ALERT_3_C	Low	Bond Precision on	C-C Bonds	.....		0.00418	Ang.
PLAT703_ALERT_1_C	Torsion Calc	-57.26(17), Rep	-57.5(2), Dev..			1.41	Sigma
	O(2)-S(1)-N(4)-N(5)	1_555 1_555	1_555 1_555	#		1	Check
PLAT703_ALERT_1_C	Torsion Calc	-52.33(16), Rep	-52.1(2), Dev..			1.44	Sigma
	O(3)-S(1)-N(4)-C(22)	1_555 1_555	1_555 1_555	#		6	Check
PLAT703_ALERT_1_C	Torsion Calc	57.29(16), Rep	57.1(2), Dev..			1.19	Sigma
	C(8)-S(1)-N(4)-N(5)	1_555 1_555	1_555 1_555	#		11	Check
PLAT703_ALERT_1_C	Torsion Calc	10.7(4), Rep	10.1(5), Dev..			1.50	Sigma
	N(1)-N(2)-C(23)-C(24)	1_555 1_555	1_555 1_555	#		17	Check
PLAT703_ALERT_1_C	Torsion Calc	-176.96(18), Rep	-177.2(2), Dev..			1.33	Sigma
	C(22)-N(4)-N(5)-C(10)	1_555 1_555	1_555 1_555	#		19	Check
PLAT703_ALERT_1_C	Torsion Calc	175.2(2), Rep	174.8(3), Dev..			2.00	Sigma
	C(10)-C(2)-C(11)-C(14)	1_555 1_555	1_555 1_555	#		32	Check
PLAT703_ALERT_1_C	Torsion Calc	-175.9(2), Rep	-175.6(3), Dev..			1.50	Sigma
	C(10)-C(2)-C(12)-C(21)	1_555 1_555	1_555 1_555	#		35	Check
PLAT703_ALERT_1_C	Torsion Calc	-1.3(4), Rep	-0.8(5), Dev..			1.25	Sigma
	C(11)-C(2)-C(12)-C(21)	1_555 1_555	1_555 1_555	#		38	Check
PLAT703_ALERT_1_C	Torsion Calc	0.5(4), Rep	-0.1(4), Dev..			1.50	Sigma
	C(12)-C(2)-C(11)-C(14)	1_555 1_555	1_555 1_555	#		39	Check
PLAT703_ALERT_1_C	Torsion Calc	178.8(2), Rep	179.1(3), Dev..			1.50	Sigma
	N(1)-C(18)-C(20)-C(17)	1_555 1_555	1_555 1_555	#		50	Check

### Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature ..... (K)	293 Check
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 !

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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28 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
 9 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

### **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__144149_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*1.00
RESPONSE: ...
;
_vrf_REFLT02__144149_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__144149_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
```

```

_vrf_DIFMX02__144149_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT098__144149_1
;
PROBLEM: Large Reported Min. (Negative) Residual Density -2.55 eA-3
RESPONSE: ...
;
_vrf_PLAT230__144149_1
;
PROBLEM: Hirshfeld Test Diff for S1 --O2 . 10.2 s.u.
RESPONSE: ...
;
_vrf_PLAT245__144149_1
;
PROBLEM: U(iso) H2 Smaller than U(eq) C17 by 0.064 Ang**2
RESPONSE: ...
;
_vrf_PLAT360__144149_1
;
PROBLEM: Short C(sp3)-C(sp3) Bond C19 - C25 . 1.30 Ang.
RESPONSE: ...
;
_vrf_PLAT166__144149_1
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged .... H1 Note
RESPONSE: ...
;
_vrf_PLAT220__144149_1
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
RESPONSE: ...
;
_vrf_PLAT222__144149_1
;
PROBLEM: NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 9.9 Ratio
RESPONSE: ...
;
_vrf_PLAT241__144149_1
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of N1 Check
RESPONSE: ...
;
_vrf_PLAT242__144149_1
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
RESPONSE: ...
;
_vrf_PLAT340__144149_1
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00418 Ang.
RESPONSE: ...
;
_vrf_PLAT703__144149_1
;

```

PROBLEM: Torsion Calc -57.26(17), Rep -57.5(2), Dev.. 1.41 Sigma  
RESPONSE: ...  
;  
# end Validation Reply Form

**PLATON version of 02/02/2025; check.def file version of 02/02/2025**

Datablock \_144149\_1 - ellipsoid plot

