

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 = 0.0043 A	Wavelength=1.54187	
Cell:	a=7.1655 (3)	b=11.9214 (5)	c=19.5707 (9)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

```
Correction method= # Reported T Limits: Tmin=0.604 Tmax=0.853
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0550( 13295)      wR2(reflections)=
S = 1.119                          0.0814( 13381)
Npar= 262
```

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 $< -0.1 \cdot Z_{\text{MAX}} \cdot 2.00$
_refine_diff_density_min given = -4.970
Test value = -3.200

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 7.02 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 -4.97 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

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 = 2751
Number of reflections greater than sigma threshold = 13295

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	S1	--N4	.	9.6 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	S1	--C1	.	7.1 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C10	--C13	.	7.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C13	--C22	.	7.7 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C14	--C19	.	14.0 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C18	--C23	.	8.2 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C20	--C22	.	9.2 s.u.
PLAT245_ALERT_2_B	U(iso) H3	Smaller than U(eq)	C23	by	0.080 Ang**2
PLAT245_ALERT_2_B	U(iso) H9	Smaller than U(eq)	N6	by	0.060 Ang**2
PLAT703_ALERT_1_B	Torsion Calc	174.4(2), Rep	173.9(3), Dev..		2.50 Sigma
	C(10-C(13-C(15-C(18	1_555 1_555 1_555 1_555	#	42	Check



Alert level C

DIFMN03_ALERT_1_C The minimum difference density is $< -0.1 \cdot Z_{\text{MAX}} \cdot 0.75$
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is $> 0.1 \cdot Z_{\text{MAX}} \cdot 0.75$

The relevant atom site should be identified.

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low	0.967	Why?
PLAT034_ALERT_1_C	No Flack Parameter Given.	Z > Si, NonCentro	Please Do !
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio	(Zmax < 18)	6.42 Note
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
PLAT222_ALERT_3_C	NonSolvent Resd 1	H Uiso(max)/Uiso(min) Range	10.0	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	S1 --O2	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C16 --C21	.	5.7 s.u.
PLAT245_ALERT_2_C	U(iso) H2	Smaller than U(eq) C15	by	0.011 Ang**2
PLAT245_ALERT_2_C	U(iso) H5	Smaller than U(eq) C22	by	0.040 Ang**2
PLAT245_ALERT_2_C	U(iso) H6	Smaller than U(eq) C12	by	0.016 Ang**2
PLAT340_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00425 Ang.
PLAT703_ALERT_1_C	Torsion Calc	-174.69(15), Rep -174.43(18), Dev..		1.73 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	152.41(13), Rep 152.26(19), Dev..		1.15 Sigma
	O(2)-S(1)-C(1)-C(9)	1_555 1_555 1_555 1_555	#	4 Check
PLAT703_ALERT_1_C	Torsion Calc	-81.82(19), Rep -82.1(2), Dev..		1.47 Sigma
	O(3)-S(1)-N(4)-C(17)	1_555 1_555 1_555 1_555	#	6 Check
PLAT703_ALERT_1_C	Torsion Calc	-167.0(2), Rep -167.3(3), Dev..		1.50 Sigma
	C(16)-N(1)-N(6)-C(8)	1_555 1_555 1_555 1_555	#	14 Check
PLAT703_ALERT_1_C	Torsion Calc	42.2(2), Rep 41.9(3), Dev..		1.50 Sigma
	S(1)-N(4)-N(5)-C(10)	1_555 1_555 1_555 1_555	#	15 Check
PLAT703_ALERT_1_C	Torsion Calc	1.8(3), Rep 2.2(4), Dev..		1.33 Sigma
	N(4)-N(5)-C(10)-C(9)	1_555 1_555 1_555 1_555	#	17 Check
PLAT703_ALERT_1_C	Torsion Calc	178.03(16), Rep 178.2(2), Dev..		1.06 Sigma
	N(4)-N(5)-C(10)-C(13)	1_555 1_555 1_555 1_555	#	18 Check
PLAT703_ALERT_1_C	Torsion Calc	179.08(18), Rep 179.3(2), Dev..		1.22 Sigma
	C(9)-C(1)-C(8)-N(6)	1_555 1_555 1_555 1_555	#	27 Check
PLAT703_ALERT_1_C	Torsion Calc	-175.5(2), Rep -175.2(3), Dev..		1.50 Sigma
	C(10)-C(13)-C(22)-C(20)	1_555 1_555 1_555 1_555	#	43 Check
PLAT703_ALERT_1_C	Torsion Calc	-3.7(4), Rep -4.2(5), Dev..		1.25 Sigma
	C(22)-C(13)-C(15)-C(18)	1_555 1_555 1_555 1_555	#	45 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 !
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		3 Units

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

19 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
9 ALERT type 4 Improvement, methodology, query or suggestion
3 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__143768_2
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143768_2
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143768_2
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
```

```

;
_vrf_PLAT230__143768_2
;
PROBLEM: Hirshfeld Test Diff for      S1      --N4      .      9.6 s.u.
RESPONSE: ...
;
_vrf_PLAT245__143768_2
;
PROBLEM: U(iso) H3      Smaller than U(eq) C23      by      0.080 Ang**2
RESPONSE: ...
;
_vrf_PLAT703__143768_2
;
PROBLEM: Torsion Calc      174.4(2), Rep      173.9(3), Dev..      2.50 Sigma
RESPONSE: ...
;
_vrf_PLAT029__143768_2
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.967 Why?
RESPONSE: ...
;
_vrf_PLAT034__143768_2
;
PROBLEM: No Flack Parameter Given. Z > Si, NonCentro ....      Please Do !
RESPONSE: ...
;
_vrf_PLAT089__143768_2
;
PROBLEM: Poor Data / Parameter Ratio (Zmax < 18) .....      6.42 Note
RESPONSE: ...
;
_vrf_PLAT166__143768_2
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....      H1 Note
RESPONSE: ...
;
_vrf_PLAT222__143768_2
;
PROBLEM: NonSolvent Resd 1  H      Uiso(max)/Uiso(min) Range      10.0 Ratio
RESPONSE: ...
;
_vrf_PLAT340__143768_2
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00425 Ang.
RESPONSE: ...
;
# end Validation Reply Form

```

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

