

R(reflections)= 0.0380( 12220)	wR2(reflections)= 0.0550( 12252)
S = 1.043	Npar= 375

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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

DIFMN02\_ALERT\_2\_A The minimum difference density is  $< -0.1 \times Z_{\text{MAX}} \times 2.00$   
\_refine\_diff\_density\_min given = -2.920  
Test value = -1.600

**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 3.62 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 -2.92 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 -1.1(3), Rep -2.1(4), Dev.. 3.33 Sigma  
C(20-C(26-C(30-C(28 1\_555 1\_555 1\_555 1\_555 # 58 Check

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

PLAT703\_ALERT\_1\_A Torsion Calc 0.9(3), Rep 2.0(4), Dev.. 3.67 Sigma  
C(22-C(28-C(30-C(26 1\_555 1\_555 1\_555 1\_555 # 60 Check

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

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### 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 = 4137  
Number of reflections greater than sigma threshold = 12220

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C22 --C28 . 8.1 s.u.  
PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for O2 --C8 . 13.9 s.u.

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O5	--C8	.	11.8 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C13	--C25	.	8.1 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C27	--C32	.	10.0 s.u.
PLAT351_ALERT_3_B	Long C-H (X0.96,N1.08A)	C30	- H23	.	1.17 Ang.
PLAT703_ALERT_1_B	Torsion Calc	177.60(13), Rep	177.25(18), Dev..		2.69 Sigma
	C(12-N(1)-C(11-C(6)	1_555 1_555 1_555 1_555	#	5	Check

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

PLAT703_ALERT_1_B	Torsion Calc	0.8(3), Rep	1.5(4), Dev..		2.33 Sigma
	C(10-C(20-C(26-C(30	1_555 1_555 1_555 1_555	#	53	Check

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

PLAT703_ALERT_1_B	Torsion Calc	-0.5(3), Rep	-1.3(4), Dev..		2.67 Sigma
	C(10-C(22-C(28-C(30	1_555 1_555 1_555 1_555	#	55	Check

**Author Response: The structre 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	_diffn_measured_fraction_theta_full value Low	0.973 Why?
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	6.40 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 ....	H11 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H12 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H13 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H14 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H16 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H17 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H18 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H19 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H22 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H23 Note
PLAT166_ALERT_4_C	S.U's Given on Coordinates for Calc-flagged ....	H24 Note
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	5.9 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C19 --C24 . 6.4 s.u.

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C21	--C29	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O4	--C14	.	5.4 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C16	--C31	.	6.0 s.u.
PLAT245_ALERT_2_C	U(iso) H1	Smaller than U(eq)	C18	by	0.014 Ang**2
PLAT245_ALERT_2_C	U(iso) H11	Smaller than U(eq)	C11	by	0.023 Ang**2
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A)	C15	- H3	.	1.14 Ang.
PLAT703_ALERT_1_C	Torsion Calc	-59.00(17), Rep	-59.2(2), Dev..		1.18 Sigma
	C(23-N(1)-C(11-C(6)	1_555	1_555	1_555	1_555 # 6 Check

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

PLAT703_ALERT_1_C	Torsion Calc	-44.32(13), Rep	-44.48(17), Dev..		1.23 Sigma
	C(18-C(6)-C(7)-O(1)	1_555	1_555	1_555	1_555 # 12 Check

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

PLAT703_ALERT_1_C	Torsion Calc	-160.70(12), Rep	-160.91(16), Dev..		1.75 Sigma
	C(18-C(6)-C(7)-C(10	1_555	1_555	1_555	1_555 # 14 Check

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

PLAT703_ALERT_1_C	Torsion Calc	-136.84(15), Rep	-137.0(2), Dev..		1.07 Sigma
	C(6)-C(7)-C(9)-C(21	1_555	1_555	1_555	1_555 # 22 Check

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

PLAT703_ALERT_1_C	Torsion Calc	163.71(13), Rep	163.92(18), Dev..		1.62 Sigma
	O(5)-C(8)-C(14-O(4)	1_555	1_555	1_555	1_555 # 31 Check

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

PLAT703_ALERT_1_C	Torsion Calc	179.17(16), Rep	178.9(2), Dev..		1.69 Sigma
	C(7)-C(10-C(20-C(26	1_555	1_555	1_555	1_555 # 37 Check

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

PLAT703_ALERT_1_C	Torsion Calc	-179.30(15), Rep	-179.0(2), Dev..		2.00 Sigma
	C(7)-C(10-C(22-C(28	1_555	1_555	1_555	1_555 # 38 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc 0.3(2), Rep 0.6(3), Dev.. 1.50 Sigma  
C(20-C(10-C(22-C(28 1\_555 1\_555 1\_555 1\_555 # 39 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc -0.4(2), Rep -0.8(3), Dev.. 2.00 Sigma  
C(22-C(10-C(20-C(26 1\_555 1\_555 1\_555 1\_555 # 40 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc -101.75(17), Rep -102.0(2), Dev.. 1.47 Sigma  
C(16-C(13-C(14-C(8) 1\_555 1\_555 1\_555 1\_555 # 43 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc -178.41(17), Rep -178.6(2), Dev.. 1.12 Sigma  
C(14-C(13-C(25-C(27 1\_555 1\_555 1\_555 1\_555 # 44 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc 0.1(3), Rep 0.6(4), Dev.. 1.67 Sigma  
C(13-C(16-C(31-C(32 1\_555 1\_555 1\_555 1\_555 # 50 Check

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

PLAT703\_ALERT\_1\_C Torsion Calc 0.2(3), Rep -0.4(4), Dev.. 2.00 Sigma  
C(16-C(31-C(32-C(27 1\_555 1\_555 1\_555 1\_555 # 61 Check

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



#### **Alert level G**

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....	1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)	293 Check

PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1	.	107.7 Degree
PLAT791_ALERT_4_G	Model has Chirality at C6	(Sohnke SpGr)	S Verify
PLAT791_ALERT_4_G	Model has Chirality at C14	(Sohnke 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	No Info/Value for _atom_sites_solution_primary	.	Please Do !

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

26 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
15 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
20 ALERT type 4 Improvement, methodology, query or suggestion  
3 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_REFLT02__138074_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__138074_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__138074_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT230__138074_1
;
PROBLEM: Hirshfeld Test Diff for      C22      --C28      .      8.1 s.u.
RESPONSE: ...
;
_vrf_PLAT351__138074_1
;
PROBLEM: Long      C-H (X0.96,N1.08A)  C30      - H23      .      1.17 Ang.
RESPONSE: ...
;
_vrf_PLAT029__138074_1
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.973 Why?
RESPONSE: ...
;
_vrf_PLAT042__138074_1
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT089__138074_1
;
PROBLEM: Poor Data / Parameter Ratio (Zmax < 18) .....      6.40 Note
RESPONSE: ...
;
_vrf_PLAT166__138074_1
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....      H1 Note
RESPONSE: ...
;
_vrf_PLAT222__138074_1
;
PROBLEM: NonSolvent Resd 1  H      Uiso(max)/Uiso(min) Range      5.9 Ratio
RESPONSE: ...
;
_vrf_PLAT245__138074_1
;
PROBLEM: U(iso) H1      Smaller than U(eq) C18      by      0.014 Ang**2
RESPONSE: ...
;
# end Validation Reply Form

```

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock \_138074\_1 - ellipsoid plot

