

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 = 0.0059 Å	Wavelength=1.54187	
Cell:	a=10.3705(8)	b=37.377(3)	c=10.6257(8)
	alpha=90	beta=104.647(3)	gamma=90
Temperature:	293 K		

```
Correction method= # Reported T Limits: Tmin=0.706 Tmax=0.884
AbsCorr = MULTI-SCAN
```

```
R(reflections)= 0.0767( 20535)      wR2(reflections)=
S = 1.074                          0.1030( 20815)
Npar= 547
```

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*ZMAX*2.00
_refine_diff_density_min given = -12.600
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 5.03 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 -12.60 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 60.6(3), Rep 59.5(5), Dev.. 3.67 Sigma
C(39-N(2)-C(45-C(3) 1_555 1_555 1_555 1_555 # 46 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 = 7615
Number of reflections greater than sigma threshold = 20535

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	Cl1	--C29	.	8.3 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N13	--C28	.	8.3 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	S1	--O6	.	7.5 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O9	--C41	.	7.2 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O9	--C54	.	7.8 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C22	--C33	.	7.7 s.u.
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of				C49 Check
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of				C55 Check
PLAT360_ALERT_2_B	Short C(sp3)-C(sp3) Bond	C49	- C56	.	1.30 Ang.
PLAT360_ALERT_2_B	Short C(sp3)-C(sp3) Bond	C54	- C55	.	1.30 Ang.

PLAT410_ALERT_2_B	Short Intra H...H Contact	H23	..H36	.	1.87 Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_B	Short Intra H...H Contact	H24	..H35	.	1.87 Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_B	Short Intra H...H Contact	H31	..H34	.	1.88 Ang.
			x,y,z =	1_555	Check
PLAT410_ALERT_2_B	Short Intra H...H Contact	H32	..H33	.	1.89 Ang.
			x,y,z =	1_555	Check
PLAT703_ALERT_1_B	Torsion Calc	178.5(2), Rep	177.9(3), Dev..		3.00 Sigma
	O(6)-S(1)-N(1)-C(24)	1_555	1_555	1_555	1_555 # 1 Check

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

PLAT703_ALERT_1_B	Torsion Calc	178.8(4), Rep	179.8(5), Dev..		2.50 Sigma
	C(49)-O(12)-C(43)-C(30)	1_555	1_555	1_555	1_555 # 35 Check

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

PLAT703_ALERT_1_B	Torsion Calc	-54.1(3), Rep	-53.2(5), Dev..		3.00 Sigma
	C(34)-N(2)-C(45)-C(20)	1_555	1_555	1_555	1_555 # 44 Check

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

PLAT703_ALERT_1_B	Torsion Calc	-179.1(3), Rep	-178.4(5), Dev..		2.33 Sigma
	C(32)-C(2)-C(24)-N(1)	1_555	1_555	1_555	1_555 # 73 Check

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

PLAT703_ALERT_1_B	Torsion Calc	-99.9(4), Rep	-99.0(5), Dev..		2.25 Sigma
	C(26)-C(3)-C(45)-N(2)	1_555	1_555	1_555	1_555 # 78 Check

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

PLAT703_ALERT_1_B	Torsion Calc	-49.6(5), Rep	-50.7(7), Dev..		2.20 Sigma
	C(38)-C(3)-C(45)-C(20)	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.

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 . 0.977 Why?

PLAT213_ALERT_2_C Atom C49 has ADP max/min Ratio 3.9 prolat

PLAT213_ALERT_2_C Atom C55 has ADP max/min Ratio 3.5 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.4 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 4.2 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for S2 --O7 . 5.7 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for S2 --N13 . 7.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for S2 --C38 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for N2 --C34 . 6.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C20 --C28 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C20 --C45 . 7.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C21 --C38 . 6.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C28 --C37 . 6.2 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C30 --C43 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C34 --C46 . 5.2 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C42 --C43 . 5.8 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for O8 --C55 . 5.1 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 --C24 . 6.7 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for N3 --C35 . 5.7 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C32 --C41 . 5.2 s.u.

PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C56 . 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C49 --C56 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C54 --C55 . 0.16 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C44 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C53 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O12 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O8 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00594 Ang.

PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS <= 51 Ang**3

PLAT703_ALERT_1_C Torsion Calc -51.8(3), Rep -52.4(4), Dev.. 2.00 Sigma

O(10)-S(1)-N(1)-C(24) 1_555 1_555 1_555 1_555 # 5 Check

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

PLAT703_ALERT_1_C Torsion Calc 61.3(3), Rep 60.7(4), Dev.. 2.00 Sigma

C(25)-S(1)-N(1)-C(24) 1_555 1_555 1_555 1_555 # 11 Check

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

PLAT703_ALERT_1_C Torsion Calc 142.9(2), Rep 142.5(3), Dev.. 2.00 Sigma
O(5)-S(2)-N(13-C(31) 1_555 1_555 1_555 1_555 # 14 Check

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

PLAT703_ALERT_1_C Torsion Calc 98.4(3), Rep 97.9(5), Dev.. 1.67 Sigma
O(5)-S(2)-C(38-C(3) 1_555 1_555 1_555 1_555 # 15 Check

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

PLAT703_ALERT_1_C Torsion Calc -76.2(3), Rep -75.6(4), Dev.. 2.00 Sigma
O(5)-S(2)-C(38-C(21) 1_555 1_555 1_555 1_555 # 16 Check

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

PLAT703_ALERT_1_C Torsion Calc -133.9(3), Rep -134.5(5), Dev.. 2.00 Sigma
O(7)-S(2)-C(38-C(3) 1_555 1_555 1_555 1_555 # 19 Check

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

PLAT703_ALERT_1_C Torsion Calc 51.5(3), Rep 52.0(5), Dev.. 1.67 Sigma
O(7)-S(2)-C(38-C(21) 1_555 1_555 1_555 1_555 # 20 Check

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

PLAT703_ALERT_1_C Torsion Calc -17.8(4), Rep -18.5(6), Dev.. 1.75 Sigma
N(13-S(2)-C(38-C(3) 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 167.6(2), Rep 168.0(4), Dev.. 2.00 Sigma
N(13-S(2)-C(38-C(21) 1_555 1_555 1_555 1_555 # 22 Check

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

PLAT703_ALERT_1_C Torsion Calc 67.2(3), Rep 67.6(4), Dev.. 1.33 Sigma
C(38-S(2)-N(13-C(28) 1_555 1_555 1_555 1_555 # 23 Check

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

PLAT703_ALERT_1_C Torsion Calc 12.0(8), Rep 11.1(12), Dev.. 1.12 Sigma
C(32-O(8)-C(55-C(54 1_555 1_555 1_555 1_555 # 28 Check

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

PLAT703_ALERT_1_C Torsion Calc 172.7(4), Rep 173.4(6), Dev.. 1.75 Sigma
C(54-O(9)-C(41-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 -75.3(4), Rep -74.7(6), Dev.. 1.50 Sigma
S(1)-N(1)-C(24-C(22 1_555 1_555 1_555 1_555 # 38 Check

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

PLAT703_ALERT_1_C Torsion Calc -83.8(4), Rep -84.3(6), Dev.. 1.25 Sigma
C(51-N(1)-C(24-C(2) 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 -44.5(3), Rep -44.1(5), Dev.. 1.33 Sigma
C(39-N(2)-C(34-C(46 1_555 1_555 1_555 1_555 # 42 Check

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

PLAT703_ALERT_1_C Torsion Calc -166.9(3), Rep -167.4(4), Dev.. 1.67 Sigma
C(45-N(2)-C(34-C(46 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_C Torsion Calc 174.9(3), Rep 174.5(4), Dev.. 1.33 Sigma
C(35-N(3)-C(33-C(1) 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_C Torsion Calc -56.8(4), Rep -57.3(6), Dev.. 1.25 Sigma
C(35-N(3)-C(33-C(22 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_C Torsion Calc -174.8(3), Rep -175.2(5), Dev.. 1.33 Sigma
C(52-N(3)-C(33-C(22 1_555 1_555 1_555 1_555 # 54 Check

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

PLAT703_ALERT_1_C Torsion Calc -179.8(3), Rep -179.4(4), Dev.. 1.33 Sigma
C(33-C(1)-C(25-C(27 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 -174.0(3), Rep -173.5(4), Dev.. 1.67 Sigma
C(26-C(3)-C(38-S(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 0.1(5), Rep -0.6(8), Dev.. 1.40 Sigma
C(26-C(3)-C(38-C(21 1_555 1_555 1_555 1_555 # 76 Check

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

PLAT703_ALERT_1_C Torsion Calc 134.8(3), Rep 134.4(5), Dev.. 1.33 Sigma
C(26-C(3)-C(45-C(20 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 175.5(3), Rep 175.0(5), Dev.. 1.67 Sigma
C(45-C(3)-C(26-C(17 1_555 1_555 1_555 1_555 # 80 Check

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

PLAT703_ALERT_1_C Torsion Calc 10.4(5), Rep 11.4(9), Dev.. 2.00 Sigma
C(45-C(3)-C(38-S(2) 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 1.0(5), Rep 0.4(7), Dev.. 1.20 Sigma
C(28-C(20-C(30-C(43 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 -58.3(4), Rep -58.8(5), Dev.. 1.25 Sigma
C(28-C(20-C(45-N(2) 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 66.7(5), Rep 67.3(6), Dev.. 1.20 Sigma
C(28-C(20-C(45-C(3) 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 118.5(4), Rep 117.8(5), Dev.. 1.75 Sigma
C(30-C(20-C(45-N(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 -116.6(4), Rep -116.1(5), Dev.. 1.25 Sigma
C(30-C(20-C(45-C(3) 1_555 1_555 1_555 1_555 # 96 Check

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

PLAT703_ALERT_1_C Torsion Calc -175.9(4), Rep -176.4(5), Dev.. 1.25 Sigma
C(45-C(20-C(30-C(43 1_555 1_555 1_555 1_555 # 97 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 2.5(9), Dev.. 1.60 Sigma
C(29-C(21-C(38-C(3) 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 179.2(3), Rep 178.8(4), Dev.. 1.33 Sigma
C(38-C(21-C(29-CL(1 1_555 1_555 1_555 1_555 # 100 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(6), Rep -0.7(8), Dev.. 1.17 Sigma
C(33-C(22-C(24-N(1 1_555 1_555 1_555 1_555 # 104 Check

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

PLAT703_ALERT_1_C Torsion Calc 1.6(6), Rep 0.6(8), Dev.. 1.67 Sigma
C(24-C(22-C(36-C(41 1_555 1_555 1_555 1_555 # 106 Check

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

PLAT703_ALERT_1_C Torsion Calc 121.5(4), Rep 121.0(5), Dev.. 1.25 Sigma
C(36-C(22-C(33-N(3 1_555 1_555 1_555 1_555 # 110 Check

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

PLAT703_ALERT_1_C Torsion Calc 174.8(3), Rep 174.4(4), Dev.. 1.33 Sigma
S(1)-C(25-C(27-C(40 1_555 1_555 1_555 1_555 # 112 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(6), Rep -1.3(7), Dev.. 1.67 Sigma
C(1)-C(25-C(27-C(40 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_C Torsion Calc -179.0(3), Rep -178.5(4), Dev.. 1.67 Sigma
C(25-C(27-C(40-CL(3 1_555 1_555 1_555 1_555 # 114 Check

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

PLAT703_ALERT_1_C Torsion Calc 1.9(6), Rep 3.0(9), Dev.. 1.83 Sigma
C(20-C(30-C(43-C(42 1_555 1_555 1_555 1_555 # 119 Check

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

PLAT703_ALERT_1_C Torsion Calc -179.7(4), Rep 179.5(5), Dev.. 2.00 Sigma
O(8)-C(32)-C(41)-C(36) 1_555 1_555 1_555 1_555 # 121 Check

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

PLAT703_ALERT_1_C Torsion Calc 178.0(4), Rep 178.8(5), Dev.. 2.00 Sigma
C(2)-C(32)-C(41)-O(9) 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 -0.5(6), Rep 0.4(8), Dev.. 1.50 Sigma
C(22)-C(36)-C(41)-C(32) 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 178.7(4), Rep 178.2(5), Dev.. 1.25 Sigma
O(1)-C(42)-C(43)-C(30) 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.

PLAT703_ALERT_1_C Torsion Calc -4.0(7), Rep -5.1(9), Dev.. 1.57 Sigma
C(37)-C(42)-C(43)-C(30) 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_C Torsion Calc 6.6(4), Rep 5.9(6), Dev.. 1.75 Sigma
C(35)-C(50)-C(53)-C(52) 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.

PLAT703_ALERT_1_C Torsion Calc -30.0(4), Rep -29.5(6), Dev.. 1.25 Sigma
N(3)-C(52)-C(53)-C(50) 1_555 1_555 1_555 1_555 # 141 Check

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

PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(5)	Senseless s.u.
C(2)	-H(1)	1_555	1_555	# 34 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(6)	Senseless s.u.
C(17)	-H(2)	1_555	1_555	# 40 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(5)	Senseless s.u.
C(21)	-H(3)	1_555	1_555	# 46 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(4)	Senseless s.u.
C(26)	-H(4)	1_555	1_555	# 51 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(5)	Senseless s.u.
C(27)	-H(5)	1_555	1_555	# 53 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(5)	Senseless s.u.
C(36)	-H(6)	1_555	1_555	# 69 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(5)	Senseless s.u.
C(37)	-H(7)	1_555	1_555	# 71 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(6)	Senseless s.u.
C(47)	-H(8)	1_555	1_555	# 84 Check
PLAT751_ALERT_4_C Bond	Calc	0.95000, Rep	0.950(6)	Senseless s.u.
C(48)	-H(9)	1_555	1_555	# 85 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	119.1(4)	Senseless s.u.
C(24)	-C(2)	-H(1)	1_555 1_555 1_555	# 33 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	119.5(4)	Senseless s.u.
C(32)	-C(2)	-H(1)	1_555 1_555 1_555	# 34 Check
PLAT752_ALERT_4_C Angle	Calc	121.00, Rep	121.2(4)	Senseless s.u.
C(26)	-C(17)	-H(2)	1_555 1_555 1_555	# 39 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	120.1(4)	Senseless s.u.
C(29)	-C(17)	-H(2)	1_555 1_555 1_555	# 40 Check
PLAT752_ALERT_4_C Angle	Calc	121.00, Rep	120.5(4)	Senseless s.u.
C(29)	-C(21)	-H(3)	1_555 1_555 1_555	# 45 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	119.9(4)	Senseless s.u.
C(38)	-C(21)	-H(3)	1_555 1_555 1_555	# 46 Check
PLAT752_ALERT_4_C Angle	Calc	118.00, Rep	117.6(4)	Senseless s.u.
C(3)	-C(26)	-H(4)	1_555 1_555 1_555	# 57 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	119.8(4)	Senseless s.u.
C(17)	-C(26)	-H(4)	1_555 1_555 1_555	# 58 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	119.1(4)	Senseless s.u.
C(25)	-C(27)	-H(5)	1_555 1_555 1_555	# 60 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	118.9(5)	Senseless s.u.
C(40)	-C(27)	-H(5)	1_555 1_555 1_555	# 61 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	119.3(4)	Senseless s.u.
C(22)	-C(36)	-H(6)	1_555 1_555 1_555	# 99 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	119.5(5)	Senseless s.u.
C(41)	-C(36)	-H(6)	1_555 1_555 1_555	# 100 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	120.0(5)	Senseless s.u.
C(28)	-C(37)	-H(7)	1_555 1_555 1_555	# 102 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	120.2(6)	Senseless s.u.
C(42)	-C(37)	-H(7)	1_555 1_555 1_555	# 103 Check
PLAT752_ALERT_4_C Angle	Calc	117.00, Rep	117.2(5)	Senseless s.u.
C(1)	-C(47)	-H(8)	1_555 1_555 1_555	# 144 Check
PLAT752_ALERT_4_C Angle	Calc	119.00, Rep	118.9(5)	Senseless s.u.
C(48)	-C(47)	-H(8)	1_555 1_555 1_555	# 145 Check
PLAT752_ALERT_4_C Angle	Calc	120.00, Rep	119.9(5)	Senseless s.u.
C(40)	-C(48)	-H(9)	1_555 1_555 1_555	# 147 Check
PLAT752_ALERT_4_C Angle	Calc	121.00, Rep	121.4(6)	Senseless s.u.
C(47)	-C(48)	-H(9)	1_555 1_555 1_555	# 148 Check
PLAT754_ALERT_4_C Contact	Calc	3.15000, Rep	3.150(3)	Senseless s.u.
CL(3)	-H(3)	1_555	1_556	# 106 Check
PLAT754_ALERT_4_C Contact	Calc	3.31000, Rep	3.306(3)	Senseless s.u.

CL(3) -H(7)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.92000, Rep	2.922(5)	Senseless s.u.
O(1) -H(9)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.89000, Rep	2.887(5)	Senseless s.u.
O(1) -H(9)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.15000, Rep	3.147(4)	Senseless s.u.
O(5) -H(6)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.68000, Rep	2.683(5)	Senseless s.u.
O(5) -H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.15000, Rep	3.154(4)	Senseless s.u.
O(6) -H(1)	1_555	4_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.77000, Rep	2.772(4)	Senseless s.u.
O(7) -H(7)	1_555	3_656	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.67000, Rep	2.672(6)	Senseless s.u.
O(8) -H(2)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.49000, Rep	3.492(5)	Senseless s.u.
O(8) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.82000, Rep	2.822(5)	Senseless s.u.
O(9) -H(5)	1_555	1_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.85000, Rep	2.850(4)	Senseless s.u.
O(10) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.99000, Rep	2.988(5)	Senseless s.u.
C(2) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.20000, Rep	3.201(6)	Senseless s.u.
C(21) -H(6)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.52000, Rep	3.521(5)	Senseless s.u.
C(24) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.33000, Rep	3.330(6)	Senseless s.u.
C(28) -H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.36000, Rep	3.357(6)	Senseless s.u.
C(32) -H(2)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.19000, Rep	3.190(6)	Senseless s.u.
C(32) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.19000, Rep	3.186(5)	Senseless s.u.
C(37) -H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.54000, Rep	3.544(6)	Senseless s.u.
C(37) -H(9)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.58000, Rep	3.578(5)	Senseless s.u.
C(39) -H(6)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.40000, Rep	3.405(5)	Senseless s.u.
C(40) -H(3)	1_555	1_556	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.31000, Rep	3.309(6)	Senseless s.u.
C(42) -H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.19000, Rep	3.193(6)	Senseless s.u.
C(42) -H(9)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.51000, Rep	3.508(5)	Senseless s.u.
C(43) -H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.43000, Rep	3.430(5)	Senseless s.u.
C(44) -H(6)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.46000, Rep	3.466(5)	Senseless s.u.
C(50) -H(2)	1_555	4_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.04000, Rep	3.042(8)	Senseless s.u.
C(54) -H(5)	1_555	1_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.40000, Rep	3.397(8)	Senseless s.u.
C(55) -H(1)	1_555	4_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.34000, Rep	3.336(8)	Senseless s.u.
C(55) -H(2)	1_555	1_455	# 106 Check

PLAT754_ALERT_4_C Contact Calc	3.52000, Rep	3.515(8)	Senseless s.u.
C(56) -H(7)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.45000, Rep	3.452(7)	Senseless s.u.
C(56) -H(9)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.15000, Rep	3.154(4)	Senseless s.u.
H(1) -O(6)	1_555	4_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.40000, Rep	3.397(8)	Senseless s.u.
H(1) -C(55)	1_555	4_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.44000, Rep	3.436(5)	Senseless s.u.
H(1) -H(2)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.04000, Rep	3.038(5)	Senseless s.u.
H(1) -H(4)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.67000, Rep	2.672(6)	Senseless s.u.
H(2) -O(8)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.36000, Rep	3.357(6)	Senseless s.u.
H(2) -C(32)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.46000, Rep	3.466(5)	Senseless s.u.
H(2) -C(50)	1_555	4_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.34000, Rep	3.336(8)	Senseless s.u.
H(2) -C(55)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.44000, Rep	3.436(5)	Senseless s.u.
H(2) -H(1)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.15000, Rep	3.150(3)	Senseless s.u.
H(3) -CL(3)	1_555	1_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.40000, Rep	3.405(5)	Senseless s.u.
H(3) -C(40)	1_555	1_554	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.93000, Rep	2.932(6)	Senseless s.u.
H(3) -H(6)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.49000, Rep	3.492(5)	Senseless s.u.
H(4) -O(8)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.85000, Rep	2.850(4)	Senseless s.u.
H(4) -O(10)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.99000, Rep	2.988(5)	Senseless s.u.
H(4) -C(2)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.52000, Rep	3.521(5)	Senseless s.u.
H(4) -C(24)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.19000, Rep	3.190(6)	Senseless s.u.
H(4) -C(32)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.04000, Rep	3.038(5)	Senseless s.u.
H(4) -H(1)	1_555	1_655	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.82000, Rep	2.822(5)	Senseless s.u.
H(5) -O(9)	1_555	1_556	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.04000, Rep	3.042(8)	Senseless s.u.
H(5) -C(54)	1_555	1_556	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.15000, Rep	3.147(4)	Senseless s.u.
H(6) -O(5)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.20000, Rep	3.201(6)	Senseless s.u.
H(6) -C(21)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.58000, Rep	3.578(5)	Senseless s.u.
H(6) -C(39)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.43000, Rep	3.430(5)	Senseless s.u.
H(6) -C(44)	1_555	1_455	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.93000, Rep	2.932(6)	Senseless s.u.
H(6) -H(3)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C Contact Calc	3.31000, Rep	3.306(3)	Senseless s.u.
H(7) -CL(3)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C Contact Calc	2.77000, Rep	2.772(4)	Senseless s.u.

H(7)	-O(7)	1_555	3_656	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.52000, Rep	3.515(8)	Senseless s.u.
H(7)	-C(56)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.54000, Rep	3.536(6)	Senseless s.u.
H(7)	-H(8)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.56000, Rep	3.562(6)	Senseless s.u.
H(7)	-H(9)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.58000, Rep	3.584(6)	Senseless s.u.
H(7)	-H(9)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	2.68000, Rep	2.683(5)	Senseless s.u.
H(8)	-O(5)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.33000, Rep	3.330(6)	Senseless s.u.
H(8)	-C(28)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.19000, Rep	3.186(5)	Senseless s.u.
H(8)	-C(37)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.31000, Rep	3.309(6)	Senseless s.u.
H(8)	-C(42)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.51000, Rep	3.508(5)	Senseless s.u.
H(8)	-C(43)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.54000, Rep	3.536(6)	Senseless s.u.
H(8)	-H(7)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	2.92000, Rep	2.922(5)	Senseless s.u.
H(9)	-O(1)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	2.89000, Rep	2.887(5)	Senseless s.u.
H(9)	-O(1)	1_555	3_657	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.54000, Rep	3.544(6)	Senseless s.u.
H(9)	-C(37)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.19000, Rep	3.193(6)	Senseless s.u.
H(9)	-C(42)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.45000, Rep	3.452(7)	Senseless s.u.
H(9)	-C(56)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.56000, Rep	3.562(6)	Senseless s.u.
H(9)	-H(7)	1_555	1_555	# 106 Check
PLAT754_ALERT_4_C	Contact Calc	3.58000, Rep	3.584(6)	Senseless s.u.
H(9)	-H(7)	1_555	3_657	# 106 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
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C49 Check
PLAT793_ALERT_4_G	Model has Chirality at C33 (Centro SpGr)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C45 (Centro SpGr)	R 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 !

-
- 4 **ALERT level A** = Most likely a serious problem - resolve or explain
 21 **ALERT level B** = A potentially serious problem, consider carefully
 185 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 9 **ALERT level G** = General information/check it is not something unexpected
- 61 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
45 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
108 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__143734_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143734_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143734_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
```

```

_vrf_PLAT230__143734_1
;
PROBLEM: Hirshfeld Test Diff for    C11      --C29      .      8.3 s.u.
RESPONSE: ...
;
_vrf_PLAT241__143734_1
;
PROBLEM: High    'MainMol' Ueq as Compared to Neighbors of      C49 Check
RESPONSE: ...
;
_vrf_PLAT360__143734_1
;
PROBLEM: Short   C(sp3)-C(sp3) Bond  C49      - C56      .      1.30 Ang.
RESPONSE: ...
;
_vrf_PLAT410__143734_1
;
PROBLEM: Short Intra H...H Contact  H23      ..H36      .      1.87 Ang.
RESPONSE: ...
;
_vrf_PLAT029__143734_1
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.977 Why?
RESPONSE: ...
;
_vrf_PLAT213__143734_1
;
PROBLEM: Atom C49                      has ADP max/min Ratio .....      3.9 prolat
RESPONSE: ...
;
_vrf_PLAT220__143734_1
;
PROBLEM: NonSolvent   Resd 1   C    Ueq(max)/Ueq(min) Range      5.4 Ratio
RESPONSE: ...
;
_vrf_PLAT222__143734_1
;
PROBLEM: NonSolvent Resd 1   H    Uiso(max)/Uiso(min) Range      4.6 Ratio
RESPONSE: ...
;
_vrf_PLAT234__143734_1
;
PROBLEM: Large Hirshfeld Difference O1      --C56      .      0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT242__143734_1
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of      O1 Check
RESPONSE: ...
;
_vrf_PLAT340__143734_1
;
PROBLEM: Low Bond Precision on   C-C Bonds .....      0.00594 Ang.
RESPONSE: ...
;
_vrf_PLAT601__143734_1
;

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```
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS    <=          51 Ang**3
RESPONSE: ...
;
_vrf_PLAT751__143734_1
;
PROBLEM: Bond      Calc      0.95000, Rep      0.950(5) ..... Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT752__143734_1
;
PROBLEM: Angle     Calc      119.00, Rep      119.1(4) ..... Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT754__143734_1
;
PROBLEM: Contact Calc      3.15000, Rep      3.150(3) ..... Senseless s.u.
RESPONSE: ...
;
# end Validation Reply Form
```

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

