

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: _143519_2

Bond precision: C-C = 0.0088 Å

Wavelength=1.54187

Cell: a=6.3364(8) b=9.2356(13) c=15.0269(18)
 alpha=94.676(9) beta=95.441(7) gamma=93.115(8)
Temperature: 293 K

	Calculated	Reported
Volume	870.8(2)	870.80(19)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C19 H20 N4 O2 S	C19 H20 N4 O2 S
Sum formula	C19 H20 N4 O2 S	C19 H20 N4 O2 S
Mr	368.45	368.45
Dx, g cm ⁻³	1.405	1.405
Z	2	2
Mu (mm ⁻¹)	1.835	1.836
F000	388.0	388.0
F000'	389.73	
h,k,lmax	7,11,18	7,11,18
Nref	6830[3415]	5016
Tmin,Tmax	0.573,0.879	0.653,0.879
Tmin'	0.520	

Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.879
AbsCorr = MULTI-SCAN

Data completeness= 1.47/0.73

Theta(max)= 71.650

R(reflections)= 0.0406(7920)

wR2(reflections)=
0.0647(7963)

S = 0.940

Npar= 509

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 $< -0.1 \times Z_{MAX} \times 2.00$
_refine_diff_density_min given = -13.300
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.

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 3.363
Additional refinement cycles may be required.

Author Response: There was some convergence problem at the refinement, however there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT029_ALERT_3_A _diffraction_measured_fraction_theta_full value Low . 0.892 Why?

Author Response: Although some large-theta reflexions are too weak but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT080_ALERT_2_A Maximum Shift/Error 3.36 Why ?

Author Response: There was some convergence problem at the refinement, however 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 3.27 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 -13.30 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 -178.7(6), Rep -176.8(9), Dev.. 3.17 Sigma
N(13-C(1)-C(25-C(42 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_A Torsion Calc -0.2(9), Rep 2.6(14), Dev.. 3.11 Sigma
C(37-C(1)-C(25-C(42 1_555 1_555 1_555 1_555 # 48 Check

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

PLAT703_ALERT_1_A Torsion Calc -176.9(6), Rep -174.9(9), Dev.. 3.33 Sigma
C(41-C(3)-C(27-C(49 1_555 1_555 1_555 1_555 # 59 Check

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

PLAT703_ALERT_1_A Torsion Calc -6.4(10), Rep -9.8(15), Dev.. 3.40 Sigma
C(34-C(24-C(31-C(27 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_A Torsion Calc -6.4(9), Rep -9.9(14), Dev.. 3.89 Sigma
C(1)-C(25-C(42-C(46 1_555 1_555 1_555 1_555 # 87 Check

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

PLAT703_ALERT_1_A Torsion Calc 1.1(10), Rep 5.8(15), Dev.. 4.70 Sigma
C(40-C(25-C(42-C(45 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_A Torsion Calc 3.5(10), Rep 0.2(11), Dev.. 3.30 Sigma
C(42-C(25-C(40-C(30 1_555 1_555 1_555 1_555 # 90 Check

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

PLAT703_ALERT_1_A Torsion Calc 4.5(9), Rep 8.0(14), Dev.. 3.89 Sigma
C(3)-C(27-C(31-C(24 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_A Torsion Calc 148.7(6), Rep 145.3(10), Dev.. 5.67 Sigma
C(24-C(31-C(43-C(39 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_A Torsion Calc 54.8(7), Rep 57.0(11), Dev.. 3.14 Sigma
C(35-C(39-C(43-C(31 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_A Torsion Calc -4.6(10), Rep -7.8(14), Dev.. 3.20 Sigma
C(25-C(42-C(45-C(29 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_A Torsion Calc -150.1(6), Rep -152.1(8), Dev.. 3.33 Sigma
C(45-C(42-C(46-C(48 1_555 1_555 1_555 1_555 # 116 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 = 5016
Number of reflections greater than sigma threshold = 7920
PLAT111_ALERT_2_B ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group P-1 Check
Check Model Parameter Symmetry for Reflection Data Support
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 --O3 . 10.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N4 --N8 . 11.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C28 --C50 . 10.4 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for S2 --O5 . 11.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N1 --N2 . 13.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C16 --C20 . 11.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C29 --C45 . 7.7 s.u.
PLAT703_ALERT_1_B Torsion Calc -175.0(5), Rep -176.1(7), Dev.. 2.20 Sigma
C(19-N(4)-N(8)-C(21 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 178.6(5), Rep 179.9(6), Dev.. 2.60 Sigma
N(5)-N(10)-C(49)-C(27 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_B Torsion Calc -178.6(5), Rep -177.2(8), Dev.. 2.80 Sigma
N(3)-N(13)-C(1)-C(25 1_555 1_555 1_555 1_555 # 41 Check

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

PLAT703_ALERT_1_B Torsion Calc -0.9(9), Rep -3.5(14), Dev.. 2.89 Sigma
N(13)-C(1)-C(25)-C(40 1_555 1_555 1_555 1_555 # 43 Check

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

PLAT703_ALERT_1_B Torsion Calc 177.6(6), Rep 175.8(9), Dev.. 3.00 Sigma
C(37)-C(1)-C(25)-C(40 1_555 1_555 1_555 1_555 # 47 Check

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

PLAT703_ALERT_1_B Torsion Calc -8.8(9), Rep -10.9(14), Dev.. 2.33 Sigma
C(36)-C(23)-C(26)-C(44 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 -174.3(6), Rep -173.0(9), Dev.. 2.17 Sigma
C(1)-C(25)-C(40)-C(30 1_555 1_555 1_555 1_555 # 85 Check

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

PLAT703_ALERT_1_B Torsion Calc 4.2(9), Rep 2.2(14), Dev.. 2.22 Sigma
C(3)-C(27)-C(49)-N(10 1_555 1_555 1_555 1_555 # 93 Check

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

PLAT703_ALERT_1_B Torsion Calc 4.5(9), Rep 6.9(13), Dev.. 2.67 Sigma
C(31-C(27-C(49-C(35 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_B Torsion Calc -2.7(9), Rep -5.3(14), Dev.. 2.89 Sigma
C(49-C(27-C(31-C(43 1_555 1_555 1_555 1_555 # 98 Check

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

PLAT703_ALERT_1_B Torsion Calc 178.7(6), Rep 177.4(9), Dev.. 2.17 Sigma
N(5)-C(28-C(50-C(52 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_B Torsion Calc -4.4(9), Rep -6.3(14), Dev.. 2.11 Sigma
C(2)-C(28-C(50-C(52 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_B Torsion Calc -159.5(6), Rep -157.9(8), Dev.. 2.67 Sigma
C(39-C(35-C(49-N(10 1_555 1_555 1_555 1_555 # 107 Check

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

PLAT703_ALERT_1_B Torsion Calc -51.7(7), Rep -53.7(10), Dev.. 2.86 Sigma
C(49-C(35-C(39-C(43 1_555 1_555 1_555 1_555 # 109 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(6), Rep -179.8(7), Dev.. 2.33 Sigma
C(19-C(38-C(47-C(52 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_B Torsion Calc 7.1(11), Rep 10.0(16), Dev.. 2.64 Sigma
C(28-C(50-C(52-C(47 1_555 1_555 1_555 1_555 # 120 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.

PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro Please Do !

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.71 Note

PLAT213_ALERT_2_C Atom C21 has ADP max/min Ratio 3.1 prolat

PLAT230_ALERT_2_C Hirshfeld Test Diff for N8 --C21 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C2 --C28 . 5.4 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C19 --C32 . 5.4 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C19 --C38 . 7.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C24 --C31 . 6.8 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C24 --C34 . 5.2 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C35 --C39 . 6.2 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C1 --C37 . 5.4 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C42 --C45 . 5.7 s.u.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C39 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00876 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C25 . 1.54 Ang.

PLAT414_ALERT_2_C Short Intra D-H..H-X H1 ..H18 . 1.95 Ang.

x,y,z = 1_555 Check

PLAT703_ALERT_1_C Torsion Calc 39.6(6), Rep 40.3(9), Dev.. 1.17 Sigma

O(2)-S(1)-C(2)-C(28) 1_555 1_555 1_555 1_555 # 3 Check

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

PLAT703_ALERT_1_C Torsion Calc -146.8(5), Rep -146.1(7), Dev.. 1.40 Sigma

O(2)-S(1)-C(2)-C(38) 1_555 1_555 1_555 1_555 # 4 Check

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

PLAT703_ALERT_1_C Torsion Calc 152.8(5), Rep 153.4(8), Dev.. 1.20 Sigma

N(8)-S(1)-C(2)-C(28) 1_555 1_555 1_555 1_555 # 9 Check

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

PLAT703_ALERT_1_C Torsion Calc 49.9(5), Rep 50.5(8), Dev.. 1.20 Sigma

C(2)-S(1)-N(8)-N(4) 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 -176.4(4), Rep -175.6(6), Dev.. 2.00 Sigma
C(2)-S(1)-N(8)-C(21 1_555 1_555 1_555 1_555 # 12 Check

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

PLAT703_ALERT_1_C Torsion Calc -80.2(5), Rep -79.6(7), Dev.. 1.20 Sigma
O(1)-S(2)-C(33)-C(23 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 148.9(5), Rep 149.7(7), Dev.. 1.60 Sigma
O(5)-S(2)-C(33)-C(23 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 37.3(5), Rep 38.2(8), Dev.. 1.80 Sigma
N(2)-S(2)-C(33)-C(23 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 170.7(6), Rep 169.8(9), Dev.. 1.50 Sigma
C(26)-N(1)-N(2)-C(51 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 -38.4(6), Rep -39.1(10), Dev.. 1.17 Sigma
C(19)-N(4)-N(8)-S(1) 1_555 1_555 1_555 1_555 # 34 Check

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

PLAT703_ALERT_1_C Torsion Calc -176.6(6), Rep -177.3(9), Dev.. 1.17 Sigma
C(28)-C(2)-C(38)-C(19 1_555 1_555 1_555 1_555 # 53 Check

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

PLAT703_ALERT_1_C Torsion Calc -4.7(10), Rep -5.9(15), Dev.. 1.20 Sigma
C(27-C(3)-C(41-C(34 1_555 1_555 1_555 1_555 # 57 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(9), Rep -0.3(11), Dev.. 1.44 Sigma
C(41-C(3)-C(27-C(31 1_555 1_555 1_555 1_555 # 58 Check

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

PLAT703_ALERT_1_C Torsion Calc 175.7(6), Rep 174.6(8), Dev.. 1.83 Sigma
N(3)-C(16-C(20-C(18 1_555 1_555 1_555 1_555 # 60 Check

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

PLAT703_ALERT_1_C Torsion Calc 3.4(9), Rep 2.4(12), Dev.. 1.11 Sigma
C(20-C(16-C(33-C(23 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 5.0(10), Rep 6.2(13), Dev.. 1.20 Sigma
C(36-C(18-C(20-C(16 1_555 1_555 1_555 1_555 # 67 Check

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

PLAT703_ALERT_1_C Torsion Calc -168.7(6), Rep -169.5(9), Dev.. 1.33 Sigma
N(4)-C(19-C(38-C(47 1_555 1_555 1_555 1_555 # 69 Check

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

PLAT703_ALERT_1_C Torsion Calc 10.6(9), Rep 9.3(14), Dev.. 1.44 Sigma
C(32-C(19-C(38-C(47 1_555 1_555 1_555 1_555 # 71 Check

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

PLAT703_ALERT_1_C Torsion Calc -11.8(8), Rep -13.2(12), Dev.. 1.75 Sigma
C(26-C(23-C(33-S(2) 1_555 1_555 1_555 1_555 # 72 Check

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

PLAT703_ALERT_1_C Torsion Calc -12.6(10), Rep -11.5(15), Dev.. 1.10 Sigma
C(33-C(23-C(26-N(1) 1_555 1_555 1_555 1_555 # 74 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(7), Rep -174.6(9), Dev.. 1.86 Sigma
C(26-C(23-C(36-C(18 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 165.6(7), Rep 164.6(10), Dev.. 1.43 Sigma
C(36-C(23-C(26-N(1) 1_555 1_555 1_555 1_555 # 77 Check

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

PLAT703_ALERT_1_C Torsion Calc 169.8(5), Rep 170.5(7), Dev.. 1.40 Sigma
C(36-C(23-C(33-S(2) 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 -2.1(9), Rep -0.5(11), Dev.. 1.78 Sigma
C(36-C(23-C(33-C(16 1_555 1_555 1_555 1_555 # 81 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(6), Rep 176.7(9), Dev.. 1.33 Sigma
C(40-C(25-C(42-C(46 1_555 1_555 1_555 1_555 # 89 Check

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

PLAT703_ALERT_1_C Torsion Calc -177.7(5), Rep -178.6(8), Dev.. 1.80 Sigma
C(3)-C(27-C(49-C(35 1_555 1_555 1_555 1_555 # 94 Check

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

PLAT703_ALERT_1_C Torsion Calc -173.5(6), Rep -172.3(9), Dev.. 2.00 Sigma
C(31-C(27-C(49-N(10 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 1.0(11), Rep 2.3(16), Dev.. 1.18 Sigma
C(45-C(29-C(30-C(40 1_555 1_555 1_555 1_555 # 102 Check

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

PLAT703_ALERT_1_C Torsion Calc 2.8(10), Rep 4.4(14), Dev.. 1.60 Sigma
C(24-C(34-C(41-C(3) 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 50.9(7), Rep 50.0(10), Dev.. 1.29 Sigma
C(1)-C(37-C(48-C(46 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 35.3(9), Rep 36.8(12), Dev.. 1.67 Sigma
C(25-C(42-C(46-C(48 1_555 1_555 1_555 1_555 # 115 Check

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

PLAT703_ALERT_1_C Torsion Calc -55.2(7), Rep -54.0(10), Dev.. 1.71 Sigma
C(42-C(46-C(48-C(37 1_555 1_555 1_555 1_555 # 118 Check

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

PLAT703_ALERT_1_C Torsion Calc -5.0(10), Rep -6.9(15), Dev.. 1.90 Sigma
C(38-C(47-C(52-C(50 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.



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	2	Report
	H1 H2		
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C19 H20 N4 O2 S		
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 !

18 **ALERT level A** = Most likely a serious problem - resolve or explain
26 **ALERT level B** = A potentially serious problem, consider carefully
52 **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

69 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 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
1 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__143519_2
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__143519_2
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__143519_2
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT111__143519_2
;
PROBLEM: ADDSYM Detects New (Pseudo) Centre of Symmetry .          100 %Fit
RESPONSE: ...
;
_vrf_PLAT113__143519_2
;
PROBLEM: ADDSYM Suggests Possible Pseudo/New Space Group          P-1 Check
RESPONSE: ...
;
_vrf_PLAT230__143519_2
;
PROBLEM: Hirshfeld Test Diff for      S1          --O3          .      10.0 s.u.
RESPONSE: ...
;
_vrf_PLAT034__143519_2
;
PROBLEM: No Flack Parameter Given. Z > Si, NonCentro ....      Please Do !
RESPONSE: ...
;
_vrf_PLAT089__143519_2
;
PROBLEM: Poor Data / Parameter Ratio (Zmax < 18) .....      6.71 Note
RESPONSE: ...
;
_vrf_PLAT213__143519_2
;
PROBLEM: Atom C21          has ADP max/min Ratio .....      3.1 prolat
RESPONSE: ...
;
_vrf_PLAT241__143519_2
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of          C39 Check
RESPONSE: ...
;
_vrf_PLAT340__143519_2
;
PROBLEM: Low Bond Precision on C-C Bonds .....      0.00876 Ang.
RESPONSE: ...
```

```

;
_vrf_PLAT369__143519_2
;
PROBLEM: Long C(sp2)-C(sp2) Bond C1 - C25 . 1.54 Ang.
RESPONSE: ...
;
_vrf_PLAT414__143519_2
;
PROBLEM: Short Intra D-H...H-X H1 ..H18 . 1.95 Ang.
RESPONSE: ...
;
# end Validation Reply Form

```

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

Datablock _143519_2 - ellipsoid plot

