checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGR2

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: SGGR2

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Bond precision:  C-C = 0.0430 A          Wavelength=0.71073

Cell:          a=16.8420(15)     b=19.051(2)      c=19.390(2)
               alpha=85.443(4)   beta=79.671(3)   gamma=70.858(3)
Temperature:   150 K
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	Calculated	Reported
Volume	5780.8(10)	5780.6(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H30 B4 O4 W3	C24 H30 B4 O4 W3
Sum formula	C24 H30 B4 O4 W3	C24 H30 B4 O4 W3
Mr	977.24	977.27
Dx,g cm-3	2.246	2.246
Z	8	8
Mu (mm-1)	11.936	11.937
F000	3584.0	3584.0
F000’	3567.09	
h,k,lmax	20,22,23	20,22,23
Nref	20333	20278
Tmin,Tmax	0.147,0.434	0.247,0.434
Tmin’	0.046	

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Correction method= # Reported T Limits: Tmin=0.247 Tmax=0.434
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.000

R(reflections)= 0.0880( 17986)    wR2(reflections)= 0.1952( 20278)

S = 1.135                 Npar= 899
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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.

Alert level A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.81A From W3 12.63 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.88A From C24 10.41 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.92A From W21 10.24 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.21A From C13 10.00 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.82A From W2 9.22 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03A From W2 9.18 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.69A   From W23   8.62 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.74A   From C111   8.11 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.38A   From W12   7.56 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.73A   From W22   6.52 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.31A   From W3   5.85 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.17A   From W32   5.85 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.42A   From W3   4.72 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.31A From W2 4.71 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.13A From W11 4.51 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.91A From W31 3.69 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.84A From W3 -11.47 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.87A From W2 -9.09 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.45A From W3 -4.31 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.86A From W1 -4.23 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.29A From C14 -4.23 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.88A   From W21   -3.67 eA-3

Author Response: same as above

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.49A   From W3   -3.63 eA-3

Author Response: same as above

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =   -12.441
           Test value =   -7.400

Author Response: The alert is due to spurious electron density peaks. The reason for its appearance may be inadequate absorption correction in this heavy atom structure. However the refined model is correct with respect to the atom assignment.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density   13.68 eA-3

Author Response: same as above

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density   -12.44 eA-3

Author Response: same as above

PLAT213_ALERT_2_B Atom C82   has ADP max/min Ratio .....   4.1 prolat

Author Response: due to disorder in the structure

PLAT234_ALERT_4_B Large Hirshfeld Difference C72   --C77   .   0.28 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_B Large Hirshfeld Difference C74   --C79   .   0.26 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.043 Ang.

Author Response: The structure contains large amount of disordered atom.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   35 Note

Author Response: These reflections are cut by the beam stop.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.22A   From B12   3.35 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.83A   From W32   3.17 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.34A   From C24   2.81 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.96A   From W33   2.79 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.59A   From W1   -3.50 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.24A   From W32   -3.15 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.95A   From B1   -3.11 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.40A   From W13   -3.09 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.87A   From W1   -3.05 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.69A   From W23   -2.96 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.39A   From W2   -2.93 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.37A   From W2   -2.86 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.03A   From W3   -2.78 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.27A   From B1   -2.74 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.11A   From C80   -2.74 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.83A   From W31   -2.74 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.94A   From W12   -2.56 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.75A   From C41   -2.53 eA-3

Author Response: same as above

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.70A   From W21   -2.52 eA-3

Author Response: same as above

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.
PLAT213_ALERT_2_C Atom C21   has ADP max/min Ratio .....   3.1 prolat

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio ..... 3.1 prolat

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C23 has ADP max/min Ratio ..... 3.1 prolat

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C24 has ADP max/min Ratio ..... 3.1 prolat

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio ..... 3.3 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C32 has ADP max/min Ratio ..... 3.3 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C33 has ADP max/min Ratio ..... 3.3 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C34 has ADP max/min Ratio ..... 3.3 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C35 has ADP max/min Ratio ..... 3.3 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom O83 has ADP max/min Ratio ..... 3.1 prolat

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C71 has ADP max/min Ratio ..... 3.4 oblate

Author Response: due to disorder in the structure

PLAT213_ALERT_2_C Atom C72 has ADP max/min Ratio ..... 3.4 oblate

Author Response: due to disorder in the structure

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PLAT213_ALERT_2_C Atom C73            has ADP max/min Ratio .....       3.4 oblate
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Author Response: due to disorder in the structure

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PLAT213_ALERT_2_C Atom C74            has ADP max/min Ratio .....       3.4 oblate
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Author Response: due to disorder in the structure

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PLAT213_ALERT_2_C Atom C75            has ADP max/min Ratio .....       3.4 oblate
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Author Response: due to disorder in the structure

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PLAT213_ALERT_2_C Atom C84            has ADP max/min Ratio .....       3.5 prolat
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Author Response: due to disorder in the structure

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PLAT213_ALERT_2_C Atom O112           has ADP max/min Ratio .....       3.1 oblate
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Author Response: due to disorder in the structure

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PLAT220_ALERT_2_C Non-Solvent  Resd 2  C   Ueq(max)/Ueq(min) Range        5.0 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 3  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 4  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C41      --C46      .        5.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C42      --C47      .        5.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C43      --C48      .        5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C44      --C49      .        5.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45      --C50      .        6.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference W1       --C24      .       0.16 Ang.
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Author Response: The alert is due to disorder in cyclopentadienyl moiety

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PLAT234_ALERT_4_C Large Hirshfeld Difference W1       --B1       .       0.20 Ang.
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Author Response: The alert is due to disorder in cyclopentadienyl moiety

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PLAT234_ALERT_4_C Large Hirshfeld Difference W2       --B2       .       0.17 Ang.
```

Author Response: The alert is due to disorder in cyclopentadienyl moiety

```
PLAT234_ALERT_4_C Large Hirshfeld Difference W2       --B3       .       0.19 Ang.
```

Author Response: The alert is due to disorder in cyclopentadienyl moiety

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PLAT234_ALERT_4_C Large Hirshfeld Difference W3       --B2       .       0.17 Ang.
```

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference O21 --C21 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference O23 --C23 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference O24 --C24 . 0.23 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C5 --C10 . 0.16 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C11 --C16 . 0.21 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C12 --C17 . 0.16 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C18 . 0.20 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C14 --C19 . 0.20 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C15 --C20 . 0.20 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference W11 --C52 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference O52 --C52 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C61 --C66 . 0.17 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C63 --C68 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C65 --C70 . 0.18 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C71 --C76 . 0.23 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C73 --C78 . 0.19 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference C75 --C80 . 0.23 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

PLAT234_ALERT_4_C Large Hirshfeld Difference W33 --B33 . 0.16 Ang.

Author Response: The alert is due to disorder in cyclopentadienyl moiety

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         W1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        W11 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        W13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        W21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        W23 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         92 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      6.181 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         20 Report
PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by .       1.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.76A   From C41            2.49 eA-3
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Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.29A From B1 2.45 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.58A From W13 2.44 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.75A From C84 2.44 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.41A From W3 2.37 eA-3

Author Response: These are spurious electron density peaks in this heavy atom structure which are higher than normal due to inadequate absorption correction.However the refined model is correct with respect to the atom assignment

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.30A From C104 -2.49 eA-3

Author Response: same as above

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.63A From W1 -2.39 eA-3

Author Response: same as above

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.08A From W11 -2.39 eA-3

Author Response: same as above

PLAT977_ALERT_2_C Check Negative Difference Density on H7C -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8C -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10N -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17B -0.65 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17C -1.12 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18B -0.66 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18C -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38C -0.76 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47A -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47B -0.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47C -0.56 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H69B -0.38 eA-3

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PLAT977_ALERT_2_C Check Negative Difference Density on H70A            -0.61 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H76C            -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H77B            -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H77C            -0.42 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H80A            -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H80C            -0.87 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H99A            -0.58 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     895.08 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        18 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  W1       --C22      .       5.2 s.u.
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C21 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C24 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C51 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C111 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O52      ..C63             2.93 Ang.
                                                    x,y,z  =      1_555 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
            H20B    -C20     -H20C       1.555  1.555  1.555     #  272 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
            H50A    -C50     -H50C       1.555  1.555  1.555     #  547 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.16 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
            C24 H30 B4 O4 W3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        78 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       79% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
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  23 ALERT level A = Most likely a serious problem - resolve or explain
  27 ALERT level B = A potentially serious problem, consider carefully
  88 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 114 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  30 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

PLATON version of 06/01/2019; check.def file version of 19/12/2018

Datablock SGGR2 - ellipsoid plot