checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 7

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: 7

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Bond precision:   S- C = 0.0190 A          Wavelength=0.80241

Cell:             a=16.6650(12)      b=16.8451(10)    c=18.619(2)
                  alpha=92.90(3)     beta=93.90(3)    gamma=119.49(3)
Temperature:      100 K

                  Calculated                  Reported
Volume            4517.8(16)                  4517.8(16)
Space group       P -1                        P -1
Hall group        -P 1                        -P 1
Moiety formula    C8 H24 Cl6 O Os2 S4         C8 H24 Cl6 O Os2 S4
Sum formula       C8 H24 Cl6 O Os2 S4         C8 H24 Cl6 O Os2 S4
Mr                857.67                      857.67
Dx,g cm-3         2.522                       2.522
Z                 8                           8
Mu (mm-1)         16.756                      16.756
F000              3184.0                      3184.0
F000'             3166.99
h,k,lmax          21,21,24                    21,21,24
Nref              20382                       20166
Tmin,Tmax         0.234,0.433                 0.200,0.400
Tmin'             0.150

Correction method= # Reported T Limits: Tmin=0.200 Tmax=0.400
AbsCorr = MULTI-SCAN

Data completeness= 0.989           Theta(max)= 31.205

R(reflections)= 0.0622( 17200)                wR2(reflections)=
                                              0.1527( 20166)
S = 1.041                  Npar= 800
```

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. 0.74Ang From Os1 3.69 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.77Ang From Os1 -3.63 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

Alert level B

PLAT234_ALERT_4_B Large Hirshfeld Difference S3 --C6 . 0.26 Ang.

Author Response: This is explained by the significant absorption effects, which can not be corrected completely. .

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.61Ang From Os5 3.37 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From Os3 3.33 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.01Ang From Os8 2.80 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.34Ang From Os4 2.66 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.31Ang From Os1 2.54 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.77Ang From Os5 -3.27 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.74Ang From Os3 -3.24 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.88Ang From Os1 -3.21 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.81Ang From Os5 -3.20 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.79Ang From Os6 -3.19 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.79Ang From Os4   -3.11 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.84Ang From Os8   -3.09 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Os1   -3.07 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.83Ang From Os5   -3.00 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Os7   -2.95 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.78Ang From Os8   -2.87 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.86Ang From Os3   -2.85 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.80Ang From Os5 -2.84 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.78Ang From Os7 -2.80 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.73Ang From Os7 -2.76 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.80Ang From Os6 -2.62 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.74Ang From Os3 -2.59 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.78Ang From Os2 -2.52 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.70Ang From Os8 -2.51 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

Alert level C

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PLAT234_ALERT_4_C Large Hirshfeld Difference S9       --C17      .       0.18 Ang.
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Author Response: This is explained by the significant absorption effects, which can not be corrected completely. .

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PLAT234_ALERT_4_C Large Hirshfeld Difference S9       --C18      .       0.18 Ang.
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Author Response: This is explained by the significant absorption effects, which can not be corrected completely. .

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Os6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S11 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.114 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         56 Report
                  2  0  0,  -4  2  0,  -2  2  0,   0  2  0,   2  2  0,  -2  4  0,
                 -6  6  0,  10-20  1,  -2 -2  1,   0 -2  1,   2 -2  1,  -2  0  1,
                  2  0  1,   4  0  1,  -2  2  1,   0  2  1,   2  4  1,  -4  6  1,
                 -2  6  1,  10-20  2,   0  0  2,   6  0  2,   0  2  2,   2  2  2,
                 -2 -2  3,   2  2  3,   6-18  4,  -2-12  4,   0 -2  4,   0  0  4,
                 -3 -9  5,   0 -3  5,   0 -2  5,  -2  0  5,   2  2  5,   0 -8  6,
                  6 -6  6,  -2-16  7,  -1-14  7,  -6-12  7,   2  2  7,  -7-12  8,
                 -5-11  8,   5-18  9,   5-17  9,  -3-13  9, -10 -1  9,   2  2  9,
                  7-18 10,   0-16 11,   1-10 15,  12 -5 16,  -1 -8 17,  -2  2 17,
                  0  0 18,   2  2 18,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          7 Note
                  2 -2  1,   2  0  1,   0  2  1,   6  0  2,   0  0  4,   0 -2  5,
                 -2  0  5,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.33Ang From Os6             2.47 eA-3
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Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.26Ang From Cl12            2.38 eA-3
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Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.31Ang From Os6             2.34 eA-3
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Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.52Ang From S16A 2.29 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.34Ang From Os5 2.25 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.36Ang From Os1 2.24 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27Ang From Os2 2.21 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.38Ang From Os7 2.16 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.31Ang From Os5 2.14 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From Cl4 2.06 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27Ang From Os7 1.97 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.28Ang From Os3 1.90 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From Os4 1.87 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.65Ang From Os5 1.86 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.90Ang From S3 1.86 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.25Ang From Os8 1.85 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.36Ang From Cl9 1.80 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.51Ang From Os2 1.79 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From Os8 1.78 eA-3

Author Response: There are the relatively high positive electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Os2 -2.45 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From Os2 -2.40 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.92Ang From Os8 -2.33 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.81Ang From Os4 -2.30 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.87Ang From Os1 -2.27 eA-3

Author Response: There are the relatively high negative electron density residues near the Os atoms due to the significant absorption effects, which can not be corrected completely.

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PLAT977_ALERT_2_C Check Negative Difference Density on H5B       .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6A       .      -0.46 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6C       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H21A      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24A      .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26B      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H28B      .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H32D      .      -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26E      .      -0.31 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         14 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     120.00 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.80241 Ang.
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         c         94 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group       C2/c Check
             WARNING: Disordered Atoms Excluded from Analysis
             Check Model Parameter Symmetry for Reflection Data Support
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.03 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Os5      --O3       .        5.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Os6      --O3       .        5.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of S13A       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S16A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S16B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S13B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25A       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26A       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26B       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25A       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25B       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25C       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26A       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26B       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26C       Constrained at        0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31F       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H32A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32D       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32E       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32F       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25D       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25E       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25F       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26D       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26E       Constrained at        0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26F       Constrained at        0.3 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         29% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H14B     ..H25F     .       2.06 Ang.
                                                    x,y,z  =      1_555 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Os1       (IV)      .       4.23 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Os2       (IV)      .       4.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Os3       (IV)      .       4.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Os4       (IV)      .       4.21 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Os5       (IV)      .       4.20 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Os6       (IV)      .       4.21 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         12 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        157 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         15 Note
               2  2  5,  -2 -2  1,   2  2  3,  -2 -2  3,   0  0  2,   0 -2  4,
               2  2  7,   0 14 12,  -6 -4 21, -10 -1  9,  -2 -9 21,   0 -8  6,
              -2  2 17,   2  2 18,   0  0 18,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.1 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.45 Note
            Predicted wR2: Based on SigI**2  6.24 or SHELX Weight 14.97
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  2 **ALERT level A** = Most likely a serious problem - resolve or explain
 25 **ALERT level B** = A potentially serious problem, consider carefully
 42 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 62 **ALERT level G** = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 72 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 44 ALERT type 4 Improvement, methodology, query or suggestion
  7 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 06/01/2024; check.def file version of 05/01/2024

Datablock 7 - ellipsoid plot