checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G8

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: SAlOC-1@G8

Bond precision: C-C = 0.0342 A Wavelength=1.34050

Cell: a=30.0958(6) b=30.0958(6) c=19.3547(5)
alpha=90 beta=90 gamma=90
Temperature: 113 K

	Calculated	Reported
Volume	17530.7(8)	17530.7(8)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 2(C7 H7 O), 3(C7 H8 O) [+ solv	C216 H364 Al32 N12 O110 Pb6 S12, 3(C7 H8 O), 2(C7 H7 O)
Sum formula	C251 H402 Al32 N12 O115 Pb6 S12 [+ solvent]	C251 H402 Al32 N12 O115 Pb6 S12
Mr	7919.15	7919.04
Dx,g cm-3	1.500	1.500
Z	2	2
Mu (mm-1)	5.083	5.225
F000	8024.0	8024.0
F000'	8003.89	
h,k,lmax	35,35,22	34,35,22
Nref	14970	14853
Tmin,Tmax		1.000,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = SPHERE

Data completeness= 0.992 Theta(max)= 52.048

R(reflections)= 0.1076(9225)

wR2(reflections)= 0.3415(14853)

S = 1.077 Npar= 985

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. 0.90Ang From Pb2 4.36 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.92Ang From Pb1 4.01 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.94Ang From Pb2 3.73 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb1 5.57 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb2 5.26 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb3 3.77 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

Alert level B

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C13 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C53 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N1 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N3 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C18 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03417 Ang.

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.20Ang From Pb2 3.49 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.10Ang From Pb3 3.48 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.94Ang From Pb2 3.22 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.97Ang From Pb3 2.83 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.20Ang From Pb1   2.82 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.14Ang From Pb1   2.81 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.97Ang From Pb2   2.74 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.03Ang From Pb2   2.60 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 1.34130-1.34150
           Wavelength given =    1.34050
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT082_ALERT_2_C High R1 Value ..................................       0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.34 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.62 Report
PLAT213_ALERT_2_C Atom O5              has ADP max/min Ratio .....        3.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.3 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.1 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O24 Check
```

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C32 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C46 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C52 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of S3 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C21 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C24 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C40 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C44 Check

Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.119 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O30      0.117 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O31      0.160 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H50B     ..H52B     .       1.88 Ang.
                                                    x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -4.360 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588        117 Report
               -1  3  0,  -2  4  0, -16 18  0,  22 22  0,  23 23  0,  -9 25  0,
                1 25  0,   3 31  0, -12 32  0,  -4 32  0,  14 32  0,   0  0  1,
               -2  3  1,   1  4  1,  -2  5  1,  -3  7  1,  -3  8  1,  20 22  1,
               21 22  1, -10 23  1,  -2 24  1,  12 25  1, -14 27  1,  -3 28  1,
              -16 30  1, -15 31  1, -14 31  1, -12 32  1, -11 32  1,  -1 32  1,
                4 34  1,   0  1  2,  -1  2  2,  -1  5  2,   2  7  2, -12 20  2,
               13 21  2,   4 34  2,  19 19  3,  14 24  3,  -9 25  3, -10 27  3,
              -15 28  3,   1 29  3,   2 29  3,  11 31  3,  -2 32  3, -20 22  4,
               -2 23  4,  -8 24  4, -21 27  4,   1 28  4,   2 28  4,   3 28  4,
              -17 29  4,   8 29  4,   2 32  4,   6 33  4,   0  2  5,  11 19  5,
               17 21  5,   0 22  5, -19 25  5, -12 25  5,  -9 25  5,  13 25  5,
                4 27  5,   1 29  5,   0 30  5,   3 31  5, -11 15  6,   8 17  6,
              -18 19  6,  19 19  6,  18 20  6, -20 22  6, -17 23  6, -13 23  6,
              -16 24  6,  -8 27  6,   1 27  6,   0 28  6,   1 29  6, -11 15  7,
                9 16  7,  10 16  7,  17 17  7, -16 18  7,  16 18  7, -20 21  7,
              -11 21  7, -18 22  7,  11 22  7,  -2 23  7, -16 24  7,  -8 26  7,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.08Ang From S1             2.39 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Pb3            2.02 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.87Ang From C15            1.95 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.99Ang From O8            -1.61 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.08Ang From O8      .      1.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H66       .     -0.37 eA-3
```

Alert level G

```
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        17 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         24 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
                  H9    H23
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
                  Calc: C216 H364 Al32 N12 O110 Pb6 S12, 2(C7 H7 O), 3(C7 H8 O)
                  Rep.: C216 H364 Al32 N12 O110 Pb6 S12, 3(C7 H8 O), 2
                        (C7 H7 O)
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      2.72 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     251.03 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        15 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         5 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0020 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............       0.5 Check
                  O30     C57     C58     C59     C60     C61     C62     C63
                  H57A    H57B    H57C    H60     H61     H62     H63
PLAT300_ALERT_4_G Atom Site Occupancy of C34        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C33        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H34C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35D       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O31        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C64        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C65        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C66        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C67        Constrained at       0.75 Check
```

```
PLAT300_ALERT_4_G Atom Site Occupancy of C68        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C69        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C70        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H64A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H64B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H64C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H65        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H70        Constrained at       0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         1% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       7.50 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H11A     ..H33C     .       1.97 Ang.
                                                 x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C53      ..C61      .       3.20 Ang.
                                                   x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        135 A**3
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97990 Dev...       0.01 Ang.
             C54      -H54A            1_555   1_555 ........     #  266 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             C53     -C55     -H55A       1_555  1_555  1_555     #  572 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.40 Dev...       1.40 Degree
             H64A    -C64     -H64C       1_555  1_555  1_555     #  582 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.20 Dev...       1.20 Degree
             C35     -C33     -H33C       1_555  1_555  1_555     #  610 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             H33A    -C33     -H33B       1_555  1_555  1_555     #  611 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -PB1     3_655   1_555   1_555 ......     #  219 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -PB1     4_565   1_555   1_555 ......     #  220 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -PB1     2_665   1_555   1_555 ......     #  221 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     3_655   1_555   3_655 ......     #  222 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     4_565   1_555   3_655 ......     #  223 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     3_655   1_555   4_565 ......     #  224 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     4_565   1_555   4_565 ......     #  225 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     2_665   1_555   3_655 ......     #  226 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     2_665   1_555   4_565 ......     #  227 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     2_665   1_555   2_665 ......     #  228 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     4_565   1_555   2_665 ......     #  229 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     4_565   1_555   1_555 ......     #  230 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     3_655   1_555   2_665 ......     #  231 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
```

```
             O8   -O8   -AL1     2_665   1_555   1_555 ......     #  232 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -AL1     3_655   1_555   1_555 ......     #  233 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -O8      4_565   1_555   2_665 ......     #  234 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -O8      4_565   1_555   3_655 ......     #  235 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O8   -O8   -O8      3_655   1_555   2_665 ......     #  236 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.05 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.15 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.71 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.94 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.88 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          6 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        224 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        37% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         11 Note
                0  1  2,  -1  2  2,   1 27  6,  -5 10 12,  -4 12 14,  -2  3  1,
                1  4  1,  -1  5  2,  -2  4  0,   2  7  2,   0  2  5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.284 Note
             Predicted wR2: Based on SigI**2  6.46 or SHELX Weight 31.70
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT984_ALERT_1_G The  C-f'=    0.0147 Deviates from the B&C-Value     0.0137 Check
PLAT984_ALERT_1_G The  N-f'=    0.0253 Deviates from the B&C-Value     0.0241 Check
PLAT984_ALERT_1_G The  O-f'=    0.0412 Deviates from the B&C-Value     0.0389 Check
PLAT984_ALERT_1_G The Pb-f'=   -4.2646 Deviates from the B&C-Value    -4.4950 Check
PLAT985_ALERT_1_G The Al-f"=    0.1843 Deviates from the B&C-Value     0.1873 Check
PLAT985_ALERT_1_G The Pb-f"=    7.1982 Deviates from the B&C-Value     6.8412 Check
PLAT985_ALERT_1_G The  S-f"=    0.4242 Deviates from the B&C-Value     0.4295 Check
```

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

  16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  53 ALERT type 2 Indicator that the structure model may be wrong or deficient
  23 ALERT type 3 Indicator that the structure quality may be low
  58 ALERT type 4 Improvement, methodology, query or suggestion
  10 ALERT type 5 Informative message, check
```

---

checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
```

```
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
```

```
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

Datablock SAlOC-1@G8 - ellipsoid plot