checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G3

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@G3

Bond precision: C-C = 0.0185 A Wavelength=1.34050

Cell: a=29.9222(4) b=29.9222(4) c=19.3494(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17324.3(6)	17324.3(6)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 4(C3 H7 N O) [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12, 4(C3 H7 N O)
Sum formula	C228 H392 Al32 N16 O114 Pb6 S12 [+ solvent]	C228 H392 Al32 N16 O114 Pb6 S12
Mr	7672.88	7672.77
Dx,g cm-3	1.471	1.471
Z	2	2
Mu (mm-1)	5.131	5.275
F000	7768.0	7768.0
F000'	7747.40	
h,k,lmax	35,35,22	35,33,22
Nref	14778	14729
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.997 Theta(max)= 52.046

R(reflections)= 0.0803(9937) wR2(reflections)= 0.2521(14729)

S = 1.016 Npar= 916

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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb3 3.54 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 2.75 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 C4 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 N4 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.

```
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  0.73Ang From Pb2            3.20 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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.77 Report
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        3.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.2 Ratio
PLAT241_ALERT_2_C High   '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.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 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         C5 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         C9 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 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_C High 'MainMol' Ueq as Compared to Neighbors of C31 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 C34 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 C47 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 C54 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 S2 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 N2 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 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_C Low ’MainMol’ Ueq as Compared to Neighbors of C8 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 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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 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        C19 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        C22 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        C39 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.

```
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         N1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.141 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O30      0.256 Check
PLAT317_ALERT_2_C Too many H on C in C=N Moiety in Solvent/Ion ...        C58 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01851 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C19      - C20      .       1.43 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H51B     ..H54A     .       1.94 Ang.
                                                    x,y,z  =      1_555 Check
```

```
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.136 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         47 Report
               -5  9  0,    0 12  0,  -1  2  1,  -2  4  1,   2  4  1,  -4  5  1,
                1  6  1,    3  7  1,   1  9  1,   8 10  1,   4 11  1,   0  1  2,
               -3  4  2,    6  6  2,  -1  9  2,   6 12  2,  -1 13  2,  -2  6  3,
               -8 12  3,   -1 12  3,  -3 14  3,   3  4  4,  -4  5  4,  -2  5  4,
               -1  5  4,    1  8  4,  -6 11  4,  -1  2  5,   0  5  5,  -5  9  5,
               -4  9  5,    0  4  6,   3  7  6,  -1  8  6,  10 10  6,  -7 12  6,
               -3  7  7,    7 13  7,   4  4  9,  -1  8  9,   1 10  9,  -2  8 10,
               20 23 10,   19 24 10,  14 23 11,  15 23 11,   0  0 22,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.91Ang From Pb2            2.36 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_C Check Calcd Resid. Dens.  0.93Ang From Pb1            2.29 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.  0.30Ang From Pb1            1.98 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.  0.95Ang From Pb2            1.93 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.  0.90Ang From Pb1            1.92 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.  0.92Ang From Pb1            1.61 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.

```
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From O2      .       0.69 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2BD      .      -0.34 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         26 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          25 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
              H14   H22
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.73 %
PLAT069_ALERT_1_G Atom Label Without Numerical Part ..............         Al Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.18 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         25 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          4 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
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
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              C1      C3      C36     C37     H2AA    H1A     H1B     H1C
              H2AB    H2BC    H3A     H3B     H3C     H2BD    H35A    H35B
              H35C    H35D    H36A    H36B    H36C    H37A    H37B    H37C
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         2% Note
PLAT303_ALERT_2_G Full Occupancy Atom H14       with # Connections       2.00 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C4 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C55 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H2AB     ..H4B      .       1.99 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H2BC     ..H4B      .       2.01 Ang.
                                                    x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H2BD     ..H4A      .       2.07 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H34B     ..H36B     .       1.64 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H3A      ..H38C     .       1.90 Ang.
                                               1/2-y,x,1+z  =      3_556 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H3C      ..H55B     .       2.14 Ang.
                                                -x,1-y,1-z  =      5_566 Check
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PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H33A     ..H35B     .       1.96 Ang.
                                              1-y,1/2+x,1-z  =      8_666 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H33A     ..H35C     .       2.14 Ang.
                                              1-y,1/2+x,1-z  =      8_666 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        147 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          5 Note
              Al00    H2AA    H2AB    H2BC    H2BD
PLAT721_ALERT_1_G Bond    Calc     1.00000, Rep     0.98020 Dev...       0.02 Ang.
              C1       -H1C             1_555   1_555 .......     #  197 Check
PLAT721_ALERT_1_G Bond    Calc     1.00000, Rep     0.98020 Dev...       0.02 Ang.
              C3       -H3C             1_555   1_555 .......     #  239 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.40 Dev...       1.40 Degree
              H1A     -C1      -H1C        1_555  1_555  1_555     #  437 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
              H1B     -C1      -H1C        1_555  1_555  1_555     #  438 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.30 Dev...       1.70 Degree
              C2      -C1      -H1A        1_555  1_555  1_555     #  439 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.80 Dev...       1.20 Degree
              C2      -C1      -H1B        1_555  1_555  1_555     #  440 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
              H3A     -C3      -H3B        1_555  1_555  1_555     #  523 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.40 Dev...       1.40 Degree
              H3B     -C3      -H3C        1_555  1_555  1_555     #  525 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al        (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al00      (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.73 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.81 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       281 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
               1  1  0,   0  0  1,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
               1  1  0,   0  0  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        40 Note
               0  1  2,   3  7  1,  -2  6  3,  -3  4  2,   3  4  4,  -4  5  1,
              -3  7  7,  -2  8 10,  -2  4  1,  -1  9  2,   1  8  4,  -2  5  4,
              -1  8  9,  -5  9  5,  -1  8  6,  -4  9  5,  -1 13  2,   4 11  1,
               1  9  1,   0  4  6,  -1  2  5,  -4  5  4,  -8 12  3,   3  7  6,
               6  6  2,  -7 12  6,   0  5  5,  -5  9  0,  -1  5  4,   7 13  7,
               1  6  1,   2  4  1,  -3 14  3,  -6 11  4,  10 10  6,   6 12  2,
               1 10  9,   8 10  1,   0 12  0,   4  4  9,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.5 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ         2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     5.412 Note
              Predicted wR2: Based on SigI**2  4.66 or SHELX Weight 24.81
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
```

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

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

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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@G3 - ellipsoid plot