checkCIF/PLATON report

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

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

```
Bond precision:   C-C = 0.0184 A          Wavelength=1.34050

Cell:              a=29.8347(2)      b=29.8347(2)      c=19.4324(3)
                   alpha=90          beta=90           gamma=90
Temperature:       100 K
```

	Calculated	Reported
Volume	17297.0(4)	17297.0(4)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12 [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12
Sum formula	C216 H364 Al32 N12 O110 Pb6 S12 [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12
Mr	7380.49	7380.39
Dx,g cm-3	1.417	1.417
Z	2	2
Mu (mm-1)	5.117	5.261
F000	7448.0	7448.0
F000'	7426.66	
h,k,lmax	35,35,23	35,35,23
Nref	15313	15220
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.994           Theta(max)= 52.930
```

R(reflections)= 0.0667(11995)

wR2(reflections)= 0.2078(15220)

S = 1.042 Npar= 855

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 2.43 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 C41 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.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.91Ang From Pb2 2.67 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_B Check Calcd Positive Resid. Density on       Pb2       1.88 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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.75 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        5.8 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        O21 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         C3 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         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.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C30 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 C33 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 C42 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 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 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 C7 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 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.

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 C37 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      0.148 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01837 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H5B      ..H39C     .       2.03 Ang.
                                              1-y,1/2+x,1-z  =      8_666 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H32B     ..H35C     .       2.08 Ang.
                                              1/2+y,1-x,1-z  =      7_666 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         91 Report
                2  2  0,   5  5  0,   0  6  0,   4  8  0,   8  8  0, -11 13  0,
               -6 16  0,  -5 17  0,   1 19  0,   1  3  1,   2  4  1,  -4  5  1,
               -3  5  1,   0  5  1,   5  6  1,  -5 10  1,   3 10  1,   4 12  1,
               -8 15  1,  -6 15  1,  -5 15  1, -12 16  1,   3 17  1,  -2 18  1,
                4 18  1,   0  0  2,   1  1  2,   1  2  2,  -1  3  2,   1  3  2,
               -3  5  2,  -2  5  2,   6  6  2,   4  7  2,   0  8  2,   6  8  2,
               -2 10  2,   9 10  2,  -5 11  2,   6 12  2,  12 13  2,  -5 18  2,
                0  2  3,  -2  5  3,  -2  6  3,   3  7  3,   0  8  3,  -8  9  3,
                3  9  3,  -8 10  3,   0 10  3,   2 12  3,   1  2  4,   3  4  4,
               -2  5  4,   1  6  4,  -6  7  4,  -5 10  4,  -2 11  4,   2 12  4,
                0 13  4,  -2 14  4,  -1  4  5,   5  5  5,  -2  7  5,   2  7  5,
                1  9  5,   0  0  6,  -1  3  6,  -2  4  6,  -3  5  6,  -1  6  6,
                4  6  6,   3  7  6,  -1  8  6,   2  8  6,   6  9  6,  -4 10  6,
               -2 11  6,   1  1  7,  -3  7  7,  -6  8  7,  -5  9  7,   8 11  7,
                0  1  9,  -1  6  9,  -1  8  9,  -4  6 10,  -2 19 10,  -2  3 20,
                0  0 22,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From Pb3             2.27 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.  1.05Ang From Pb2             1.82 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_C Check Calcd Resid. Dens.  1.03Ang From Pb1             1.77 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.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.83Ang From Pb2            1.76 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.  1.01Ang From Pb1            1.69 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.  0.74Ang From Pb3            1.68 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_C Check Calcd Positive Resid. Density on       Pb1       1.12 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.  0.90Ang From O4      .       1.00 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.04Ang From O3      .       0.77 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From O25     .       0.74 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.59Ang From O3      .      -0.56 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         20 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          58 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
               H14   H24
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .        2.74 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large        0.14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       15.61 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          8 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          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
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
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C3 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C4 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1 Note
          O00Y
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -PB3     3_555   1_555   1_555 ......     #  193 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -PB3     4_555   1_555   1_555 ......     #  194 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -PB3     2_555   1_555   1_555 ......     #  195 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     4_555   1_555   3_555 ......     #  196 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     2_555   1_555   4_555 ......     #  197 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     2_555   1_555   2_555 ......     #  198 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     3_555   1_555   3_555 ......     #  199 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     3_555   1_555   2_555 ......     #  200 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     2_555   1_555   3_555 ......     #  201 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     3_555   1_555   4_555 ......     #  202 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     4_555   1_555   1_555 ......     #  203 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     4_555   1_555   2_555 ......     #  204 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     3_555   1_555   1_555 ......     #  205 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     2_555   1_555   1_555 ......     #  206 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -AL8     4_555   1_555   4_555 ......     #  207 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -O25     4_555   1_555   2_555 ......     #  208 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -O25     3_555   1_555   2_555 ......     #  209 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
          O25  -O25  -O25     4_555   1_555   3_555 ......     #  210 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.83 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.77 Info
PLAT795_ALERT_4_G C-Atom in CIF Coordinate List Out-of-Sequence ..        C37 Note
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PLAT796_ALERT_4_G O-Atom in CIF Coordinate List Out-of-Sequence ..        O22 Note
PLAT797_ALERT_4_G N-Atom in CIF Coordinate List Out-of-Sequence ..         N1 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        429 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        50% Note
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 ....          1 Note
                  1  1  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         89 Note
                  0  0  1,   0  1  9,  -1  3  6,  -1  3  2,  -1  8  9,   3 17  1,
                  5  5  5,   0  6  0,  -2 19 10,   1  1  2,   9 10  2,  -2 10  2,
                  1  1  7,   8  8  0,  -5 18  2,   5  6  1,  -2  6  3,   1  2  2,
                  2  2  0,   3  7  6,   2  4  1,  -6  7  4,  -6 16  0,  -2 18  1,
                  3  9  3,  -5  9  7,   1  3  1,  -3  5  2,   6  6  2,   0  8  3,
                 -8 15  1,  -2 11  4,  -5 11  2,  -1  6  6,   3 10  1,  -2  7  5,
                  2 12  4,  -5 10  1,   1  2  4,   1  3  2,  -6 15  1,   8 11  7,
                 -3  7  7,  -1  4  5,  -4 10  6,   1  9  5,   3  4  4,  12 13  2,
                  0 10  3,  -2  5  3,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.667 Note
              Predicted wR2: Based on SigI**2  3.67 or SHELX Weight 19.95
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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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1 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
35 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
69 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
44 ALERT type 2 Indicator that the structure model may be wrong or deficient
15 ALERT type 3 Indicator that the structure quality may be low
29 ALERT type 4 Improvement, methodology, query or suggestion
10 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.
```

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   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

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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 - ellipsoid plot