checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G2

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@G2

Bond precision: C-C = 0.0265 A Wavelength=1.34050

Cell: a=29.8617(5) b=29.8617(5) c=19.1914(5)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17113.4(7)	17113.4(7)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 3(C2 H6 O S) [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12, 3(C2 H6 O S)
Sum formula	C222 H382 Al32 N12 O113 Pb6 S15 [+ solvent]	C222 H382 Al32 N12 O113 Pb6 S15
Mr	7614.88	7614.77
Dx,g cm-3	1.478	1.478
Z	2	2
Mu (mm-1)	5.298	5.442
F000	7700.0	7700.0
F000'	7680.81	
h,k,lmax	35,35,22	35,34,22
Nref	14621	14557
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.996 Theta(max)= 52.043

R(reflections)= 0.0860(8987) wR2(reflections)= 0.2836(14557)

S = 1.042 Npar= 899

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 2.44 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 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.

PLAT241_ALERT_2_B High '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.

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C25 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 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.

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 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_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 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_B Low '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.

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PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.02645 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.  1.02Ang From Pb3             3.16 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       1.90 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       Pb1       1.85 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

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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
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.28 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.41 Report
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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        5.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O7 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.

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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        C12 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
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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 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.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C20 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 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.

PLAT242_ALERT_2_C Low '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.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O14 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 C11 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 C16 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 C29 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.

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C51 Check
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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.

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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1       0.175 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        S4       0.253 Check
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C11      - C14      .        1.54 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H45A     ..H47B     .        1.94 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H22A     ..H24A     .        1.87 Ang.
                                                     x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -2.786 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         63 Report
                  1  3  0,  -2  6  0,   0  6  0,   2  6  0,   1  7  0,   8 10  0,
                  1  2  1,   4  5  1,   3  6  1,  -7  8  1,   5 10  1,   7 10  1,
                 -4 12  1,  -8 13  1,   0  1  2,  -3  4  2,   2  5  2,  -4  7  2,
                 -6  8  2,  -6  9  2,  -9 10  2,  -3 10  2,   2 10  2,  -1  2  3,
                  0  8  3,   8  8  3,   5  9  3,   3 14  3,   0  4  4,   2  5  4,
                  1  6  4,   3  8  4,  -5 10  4,   2 11  4,  -7 12  4,   0  3  5,
                  0  6  5,   5  7  5,  -6  9  5,  -3  9  5,  -1  9  5,   7 12  5,
                 -9 14  5,   1  3  6,  -6 10  6,   6 13  6,   2  6  7,   3  7  7,
                  4 10  7,  -1  4  8,   2  5  8,   4  5  8,   4  7  8,  -3 12  8,
                  1  3 10,  -5  6 10,   7 26 11,   8 26 11,   7 27 11,   7 28 11,
                  1  2 12,  -2 12 21,  -1 12 21,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.07Ang From Pb1             2.11 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.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18Ang From Pb2             2.01 eA-3
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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 Pb2 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. 0.84Ang From Pb2 1.90 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. 1.15Ang From Pb3 1.78 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. 0.94Ang 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. 0.98Ang From Pb2 1.65 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. 1.09Ang From Pb2 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.

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         32 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          34 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
              H13   H22
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.64 %
PLAT069_ALERT_1_G Atom Label Without Numerical Part .............         Al Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      21.49 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         29 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         13 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          2 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
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C6         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5AA       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5AB       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5BC       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5BD       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7B        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7C        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S4         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C56        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C57        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H56C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57C       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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       7.50 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C24 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H1A      ..H6B      .       1.63 Ang.
                                          1/2+y,1-x,1-z  =      7_666 Check
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PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H1A      ..H5BC     .       1.96 Ang.
                                              1/2+y,1-x,1-z  =      7_666 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H6C      ..H27C     .       1.92 Ang.
                                              3/2-x,1/2-y,z  =      2_655 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H44B     ..H7C      .       2.06 Ang.
                                                 3/2-y,x,1+z  =      3_656 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C6       .       3.01 Ang.
                                              1/2+y,1-x,1-z  =      7_666 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        145 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          6 Note
             Al00    O00W    H5AA    H5AB    H5BC    H5BD
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97960 Dev...       0.01 Ang.
             C7       -H7B            1_555   1_555 ........     #  221 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98020 Dev...       0.01 Ang.
             C7       -H7C            1_555   1_555 ........     #  222 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -PB1     3_655   1_555   1_555 ......     #  206 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -PB1     4_565   1_555   1_555 ......     #  207 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -PB1     2_665   1_555   1_555 ......     #  208 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     2_665   1_555   2_665 ......     #  209 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     2_665   1_555   1_555 ......     #  210 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     2_665   1_555   4_565 ......     #  211 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     4_565   1_555   2_665 ......     #  212 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     4_565   1_555   4_565 ......     #  213 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     3_655   1_555   2_665 ......     #  214 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     3_655   1_555   3_655 ......     #  215 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     3_655   1_555   4_565 ......     #  216 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     2_665   1_555   3_655 ......     #  217 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     3_655   1_555   1_555 ......     #  218 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     4_565   1_555   1_555 ......     #  219 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -AL6     4_565   1_555   3_655 ......     #  220 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -O15     3_655   1_555   2_665 ......     #  221 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -O15     4_565   1_555   2_665 ......     #  222 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O15  -O15  -O15     4_565   1_555   3_655 ......     #  223 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.01 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al        (III)     .       2.95 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 Al2       (III)     .       2.78 Info
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PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (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 .............        512 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).          1 Note
                1  1  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         54 Note
                4  7  8,   3  6  1,   4  5  8,   5  7  5,   3  8  4,   1  6  4,
               -6 10  6,   0  1  2,   4  5  1,   7 12  5,   1  3  6,  -7  8  1,
               -3  4  2,  -1  2  3,  -8 13  1,   2  5  2,   0  8  3,   2 10  2,
                8  8  3,   7 10  1,   1  2 12,   3 14  3,  -5  6 10,  -1  9  5,
               -4  7  2,   4 10  7,  -3 12  8,   2  5  8,  -5 10  4,  -6  9  2,
                2  6  7,  -9 10  2,   5  9  3,   5 10  1,  -1  4  8,  -7 12  4,
               -4 12  1,   0  6  0,  -3 10  2,  -2  6  0,   0  4  4,  -6  9  5,
               -6  8  2,   2  5  4,   3  7  7,   0  6  5,   2 11  4,   0  3  5,
                1  3 10,   6 13  6,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....        3.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      5.222 Note
             Predicted wR2: Based on SigI**2  5.43 or SHELX Weight 27.22
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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  1 **ALERT level A** = Most likely a serious problem - resolve or explain
 13 **ALERT level B** = A potentially serious problem, consider carefully
 39 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
101 **ALERT level G** = General information/check it is not something unexpected

 13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 58 ALERT type 2 Indicator that the structure model may be wrong or deficient
 20 ALERT type 3 Indicator that the structure quality may be low
 52 ALERT type 4 Improvement, methodology, query or suggestion
 11 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@G2 - ellipsoid plot