checkCIF/PLATON report

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

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-recover

Bond precision: C-C = 0.0230 A Wavelength=1.34050

Cell: a=29.8435(5) b=29.8435(5) c=19.3447(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17229.1(7)	17229.1(7)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C104 H170 Al16 N6 O55 Pb3 S6, C4 H9 [+ solvent]	C216 H358 Al32 N12 O110 Pb6 S12
Sum formula	C108 H179 Al16 N6 O55 Pb3 S6 [+ solvent]	C216 H358 Al32 N12 O110 Pb6 S12
Mr	3687.22	7374.34
Dx,g cm-3	1.421	1.421
Z	4	2
Mu (mm-1)	5.137	5.282
F000	7436.0	7436.0
F000'	7414.67	
h,k,lmax	38,38,25	36,38,24
Nref	19525	18988
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.972 Theta(max)= 60.103

R(reflections)= 0.0917(8856)

wR2(reflections)= 0.3196(18988)

S = 1.003 Npar= 887

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 2.39 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.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb2 2.28 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 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_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.

PLAT241_ALERT_2_B 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_B High '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.

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 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.

PLAT242_ALERT_2_B Low '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.

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PLAT260_ALERT_2_B Large Average Ueq of Residue Including       C19      0.309 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 ..............      0.023 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.

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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       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.

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
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..        47% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................      0.32 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.91 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       4.2 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range       3.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       6.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O3 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 C23 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 C28 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 C48 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 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_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 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 C17 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 C26 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.

PLAT242_ALERT_2_C Low ’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.

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.

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C49 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 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 C57 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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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.185 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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PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....        C22 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....        C47 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C37      - C38      .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C57      - C58      .       1.43 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H36B     ..H38B     .       1.80 Ang.
                                                    x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -14.359 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         67 Report
                  2  2  0,   3  3  0,  -2  4  0,   0  4  0,   2  4  0,  -1  5  0,
                  8 10  0,  -5 17  0,   0 22  0,   1  1  1,   1  3  1,   2  3  1,
                 -1  4  1,   1  4  1,   2  4  1,  -4  5  1,  -2  5  1,   2  5  1,
                  5  5  1,  -2  7  1,  -1  8  1,   7  8  1,  -6 15  1,   0  1  2,
                  1  2  2,   0  3  2,   1  3  2,  -2  5  2,  -1  5  2,   2  5  2,
                  3  5  2,  -5  6  2,  -3  6  2,  -4  7  2,  -1  8  2,   6  8  2,
                  6  9  2,   9 10  2,  -5 11  2,   1  2  3,  -1  4  3,  -2  5  3,
                  3  7  3,  -4  8  3,  -7 12  3,   7 13  3,   2  3  4,   3  5  5,
                  0  0  6,   2  2  6,  -1  3  6,   0  9  6,   5  9  6,  -2 10  6,
                 10 10  6,  11 11  6,  -4  5  8,   3  5  8,   2 18 10,  -5 19 10,
                  1 19 10,   2 19 10,  15 21 14,  15 22 14,  16 22 14,  15 23 14,
                 14 24 14,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From Pb3            2.49 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From Pb2            2.10 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.06Ang From Pb3            1.94 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Pb2            1.83 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.10Ang From Pb1            1.80 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From Pb2            1.76 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From Pb2            1.71 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From Pb2            1.63 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.62Ang From C45     .      -0.42 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H43A      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H45C      .      -0.33 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         30 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          50 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
              H8    H20
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C104 H170 Al16 N6 O55 Pb3 S6, C4 H9
              Rep.: C216 H358 Al32 N12 O110 Pb6 S12
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
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       0.19 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         40 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
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
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              C1      C2      C7      C8      C45     C46     H3AA    H1A
              H1B     H1C     H3AB    H2A     H2B     H2C     H3BC    H3BD
              H6AA    H6AB    H6BC    H7A     H7B     H7C     H6BD    H8A
              H8B     H8C     H45A    H45B    H45C    H46A    H46B    H46C
              H47A    H47B    C19     C20     H19A    H19B    H19C    H20A
              H20B    H20C    H21     H21A    H21B
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)          3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)         50% Note
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for          C4 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C22 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C23 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C48 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C3       - C4       .       1.51 Ang.
PLAT410_ALERT_2_G Short Intra H...H Contact  H47B     ..H48A     .       1.86 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H5A      ..H8A      .       2.13 Ang.
                                                     x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H2B      ..H56A     .       1.99 Ang.
                                               1/2-y,x,-1+z  =      3_554 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H45C     ..H58C     .       1.90 Ang.
                                              1/2+y,1-x,2-z  =      7_667 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H46B     ..H58C     .       1.99 Ang.
                                              1/2+y,1-x,2-z  =      7_667 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H19A     ..H25A     .       1.87 Ang.
                                             -1/2+y,1-x,1-z  =      7_566 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H19C     ..H23A     .       2.01 Ang.
                                                     x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H19C     ..H24B     .       1.97 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  N2       ..C19      .       2.78 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  N2       ..C20      .       2.85 Ang.
                                                     x,y,z  =      1_555 Check
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PLAT432_ALERT_2_G Short Inter X...Y Contact  N2       ..C21      .       2.94 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C22      .       2.39 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C25      .       2.94 Ang.
                                                  -1/2+y,1-x,1-z  =      7_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C23      .       3.07 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C20      ..C22      .       2.35 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C21      ..C22      .       1.91 Ang.
                                                     x,y,z  =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          8 Note
             H3AA    H3AB    H3BC    H3BD    H6AA    H6AB    H6BC    H6BD
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97990 Dev...       0.01 Ang.
             C42      -H42C            1_555   1_555 ........     #  197 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98020 Dev...       0.01 Ang.
             C1       -H1C             1_555   1_555 ........     #  232 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98010 Dev...       0.01 Ang.
             C45      -H45B            1_555   1_555 ........     #  234 Check
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97990 Dev...       0.01 Ang.
             C45      -H45C            1_555   1_555 ........     #  235 Check
PLAT722_ALERT_1_G Angle   Calc      105.00, Rep      106.70 Dev...       1.70 Degree
             C21     -C20     -H20A       1_555  1_555  1_555     #  403 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             H20B    -C20     -H20C       1_555  1_555  1_555     #  408 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      111.80 Dev...       1.80 Degree
             H19B    -C19     -H19C       1_555  1_555  1_555     #  414 Check
PLAT722_ALERT_1_G Angle   Calc      119.00, Rep      117.90 Dev...       1.10 Degree
             C47     -C46     -H46C       1_555  1_555  1_555     #  447 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             H45A    -C45     -H45B       1_555  1_555  1_555     #  511 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C22      --C21             1.91 Ang.
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set     Please Do !
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.14 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.74 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.78 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          8 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        744 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,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        462 Note
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         65 Note
                  0  1  2,  -1  8  1,   9 18 21,   5  9  6,   0 32 13,   5  5  1,
                 21 22 15,  -2  7  1,   7 16 21, -11 27 16,   1  2  2,   2  5  1,
                  7  8  1, -21 22 15, -11 35  7,   9 20 20,   9 10  2,  20 23 15,
                  1  2  3,  -5 11  2,   2  3  4,  -1  3  6,  -1  4  3,   0  9  6,
                 -1  8  2,   6  8  2,  -1  5  2,   2  5  2,   7 13  3,   3  5  5,
```

```
               10 10  6,   2  4  1,  -2 10  6,   3  5  2,  -1  4  1,  -4  5  1,
                2  4  0,   3  7  3,  -2  4  0,   1  3  2,  -1  5  0,   0  3  2,
                6  9  2,   3  3  0,  -2  5  1,   2  3  1,  11 11  6, -11 33 10,
                0 24 19,  -6 15  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....          2.7 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ       2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....        4.923 Note
             Predicted wR2: Based on SigI**2  6.49 or SHELX Weight 31.88
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
11 **ALERT level B** = A potentially serious problem, consider carefully
42 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
87 **ALERT level G** = General information/check it is not something unexpected

22 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
73 ALERT type 2 Indicator that the structure model may be wrong or deficient
21 ALERT type 3 Indicator that the structure quality may be low
14 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.
```

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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-recover - ellipsoid plot