checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G1

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@G1

```
Bond precision:   C-C = 0.0450 A          Wavelength=1.34050

Cell:             a=29.9874(5)      b=29.9874(5)      c=19.1527(6)
                  alpha=90          beta=90           gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	17223.0(8)	17223.0(8)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 3(C4 H8 O2) [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12, 3(C4 H8 O2)
Sum formula	C228 H388 Al32 N12 O116 Pb6 S12 [+ solvent]	C228 H388 Al32 N12 O116 Pb6 S12
Mr	7644.81	7644.70
Dx,g cm-3	1.474	1.474
Z	2	2
Mu (mm-1)	5.161	5.306
F000	7736.0	7736.0
F000'	7715.40	
h,k,lmax	35,35,22	35,35,22
Nref	14689	14441
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.983           Theta(max)= 52.046
```

R(reflections)= 0.1275(7541)

wR2(reflections)= 0.3416(14441)

S = 1.047 Npar= 916

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb32 2.98 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.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb3 2.76 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.

Alert level B

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C6 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 C58 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 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_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 C36 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 C39 Check

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

PLAT242_ALERT_2_B Low ’MainMol’ Ueq as Compared to Neighbors of C43 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 ..............      0.045 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.

Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 1.34130-1.34150
           Wavelength given =    1.34050
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT082_ALERT_2_C High R1 Value ..................................       0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.34 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.81 Report
PLAT213_ALERT_2_C Atom C38             has ADP max/min Ratio .....        3.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S1 Check
```

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

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

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check

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

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

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 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 C31 Check

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

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

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S2 Check

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

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check

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

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

PLAT242_ALERT_2_C Low '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.

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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.

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1       0.171 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1       0.217 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C36      - C37      .        1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C42      - C43      .        1.43 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H17B     ..H18B     .        1.92 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H57A     ..H58B     .        1.91 Ang.
                                                     x,y,z  =      1_555 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -7.726 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.065 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.714 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588        248 Report
               2  2  0,  -2  4  0,   4  4  0,  17 21  0,  -4 24  0,   8 24  0,
              -3 25  0,   7 27  0,   2 28  0,  14 28  0,  -1 29  0,  13 29  0,
              -8 30  0,  -6 30  0,  -9 31  0,  -3 31  0,  -8 32  0,   4 32  0,
               3 33  0,   0 34  0,   2 34  0,  -1 35  0,   1 35  0,   1  1  1,
               1  2  1,   1  3  1,  -2  4  1,  -4  5  1,   5  5  1,  -1  6  1,
              -3  7  1,  -2  7  1,  -1 23  1,   1 23  1,  -2 24  1,   2 24  1,
               1 25  1,  -2 26  1,  -1 26  1,   0 26  1,  -5 27  1,  -4 27  1,
               0 27  1,   7 27  1,  13 27  1,  -4 28  1,  -3 28  1,  -1 28  1,
              14 28  1,  16 28  1,  -8 29  1,  -7 29  1,  -1 29  1,  12 29  1,
              -1 30  1,   0 30  1,  13 30  1,  -9 31  1,  -5 31  1,  -4 31  1,
              -3 31  1,  -2 31  1,  -9 32  1,  -8 32  1,  -7 32  1,   3 32  1,
              -8 33  1,  -7 33  1,  -6 33  1,   2 33  1,   3 33  1,  11 33  1,
              -5 34  1,   1 34  1,   2 34  1,  -1 35  1,   0 35  1,   0  1  2,
               1  2  2,   1  5  2,  -1  6  2, -10 20  2,  14 21  2,  -1 23  2,
               0 23  2,   1 24  2,  -3 25  2,  -2 25  2,  23 25  2,  -3 26  2,
              -2 26  2,   0 26  2,  -5 27  2,  -4 27  2,   0 27  2,   1 27  2,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.24Ang From Pb1             2.09 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Pb32            1.83 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From Pb32            1.77 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.17Ang From C52             1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.20Ang From Pb32            1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Pb32            1.59 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18Ang From Pb3             1.57 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
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                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          39 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
               H5    H19
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.74 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      335.04 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         29 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
               C34     C35     H33A    H33B    H33C    H33D    H34A    H34B
               H34C    H35A    H35B    H35C
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B        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)      10.50 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1       .      106.2 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        141 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
               O0I     O0O     O013
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98020 Dev...        0.01 Ang.
               C35      -H35B          1_555   1_555 ........     #  200 Check
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97980 Dev...        0.01 Ang.
               C35      -H35C          1_555   1_555 ........     #  201 Check
PLAT721_ALERT_1_G Bond    Calc     1.00000, Rep     0.98000 Dev...        0.02 Ang.
               C34      -H34C          1_555   1_555 ........     #  204 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98020 Dev...        0.01 Ang.
               C15      -H15B          1_555   1_555 ........     #  229 Check
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97990 Dev...        0.01 Ang.
               C15      -H15C          1_555   1_555 ........     #  230 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      106.80 Dev...        1.20 Degree
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             C33     -C35     -H35B       1_555  1_555  1_555     #  486 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             H35A    -C35     -H35C       1_555  1_555  1_555     #  489 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             C33     -C34     -H34C       1_555  1_555  1_555     #  493 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             H34A    -C34     -H34B       1_555  1_555  1_555     #  494 Check
PLAT722_ALERT_1_G Angle   Calc      107.00, Rep      105.90 Dev...       1.10 Degree
             C19     -C20     -H20C       1_555  1_555  1_555     #  556 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.05 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.93 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.85 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.91 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.80 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 .............        500 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         29 Note
                0  1  2,   0  3  3,   1  1  1,   4 30  2,   5  5  1,  -1 35  2,
               -4  5  1,   1  3  1,   0 34  3,  -1  6  2,   4  4  0,   3 30  4,
                3 31  3,   1 33  3,  -1 35  0,   2  2  0,  -1 35  1,  -1 34  4,
                0 34  2,  -3  7  1, -19 20  4,   1 33  2,  -2  4  0,  -2  4  4,
               -2  7  1,  -1  6  1,   1  2  2,  -2  4  1,   0 34  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.443 Note
             Predicted wR2: Based on SigI**2  6.28 or SHELX Weight 32.63
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
   9 ALERT level B = A potentially serious problem, consider carefully
  40 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  74 ALERT level G = General information/check it is not something unexpected

  20 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  48 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
  26 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.
```

```
   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.

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Datablock SAlOC-1@G1 - ellipsoid plot