checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G7

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@G7

Bond precision: C-C = 0.0136 A Wavelength=1.34050

Cell: a=30.0205(4) b=30.0205(4) c=19.1946(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17298.8(6)	17298.8(6)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 4(C7 H6 Cl2) [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12, 4(C7 H6 Cl2)
Sum formula	C244 H388 Al32 Cl8 N12 O110 Pb6 S12 [+ solvent]	C244 H388 Al32 Cl8 N12 O110 Pb6 S12
Mr	8024.56	8024.46
Dx,g cm-3	1.541	1.541
Z	2	2
Mu (mm-1)	5.520	5.657
F000	8104.0	8104.0
F000'	8088.70	
h,k,lmax	38,38,24	38,36,24
Nref	19635	18951
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.965 Theta(max)= 60.142

R(reflections)= 0.0755(11674)

wR2(reflections)= 0.2420(18951)

S = 0.988 Npar= 1042

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.72Ang From Pb2 3.57 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 3.35 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 Pb1 3.00 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 2.45 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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.94Ang From Pb1 3.13 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_B Check Calcd Resid. Dens.  0.77Ang From Pb1            3.08 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_B Check Calcd Resid. Dens.  0.89Ang From Pb1            2.81 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_B Check Calcd Resid. Dens.  1.08Ang From Pb3            2.68 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.93 Report
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        3.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.8 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C53 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C66 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C60 Check
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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C72 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.118 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.145 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl3      0.176 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01363 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C24      - C25      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C71      - C72      .       1.38 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.431 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         82 Report
               -1  3  0,   1  3  0,   0  4  0,   2  4  0,   4  4  0,   5  5  0,
                0  6  0,   1 11  0,   0 12  0,   0  2  1,   1  2  1,   1  3  1,
               -3  4  1,  -2  4  1,   2  4  1,  -3  5  1,  -1  5  1,   1  5  1,
                5  5  1,  -1  6  1,  -4  7  1,   5  7  1,  -3  9  1,   3 14  1,
                0  1  2,   1  1  2,   2  2  2,   0  3  2,   4  4  2,  -2  5  2,
                1  5  2,   4  5  2,   2  7  2,  -3  8  2,  -2 10  2,   4 11  2,
               -5 12  2,   0 12  2,   4 12  2,  -3 13  2,   8 13  2,   9 14  2,
                0 15  2,   1  1  3,   2  2  3,   0  3  3,  -1  4  3,  -2  6  3,
                8  8  3,   1  3  4,  -1  5  4,   3  6  4,  -2  7  4,   7  9  4,
                0  2  5,  -5  6  5,   6  9  5,   0  0  6,   2  3  6,   0  4  6,
                2  4  6,   0  6  6,  -1  8  6,  -6  9  6,  -2 10  6,  -1  5  7,
               -3  7  7,  -2  5  8,  -4 11  8, -12 25 10, -11 25 10, -10 25 10,
               -8 14 11, -11 23 11, -10 23 11, -14 24 11, -13 24 11, -12 24 11,
              -17 24 13, -10 14 14,   0  0 16,   5 21 18,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.08Ang From Pb2             2.49 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.  0.75Ang From Pb2             2.27 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.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.83Ang From Pb1             2.20 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From Pb1             2.16 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.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From Pb3            2.07 eA-3
```

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Pb3            1.97 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 Pb1            1.52 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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PLAT977_ALERT_2_C Check Negative Difference Density on H19       .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23A      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38B      .      -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         34 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
              H5    H19
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .        2.42 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large        0.17 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         48 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          5 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          4 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 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
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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
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 First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0020 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
               Cl1     Cl2     C1      C2      C3      C4      C5      C6
               C7      H1A     H1B     H1C     H4      H5A     H6      Cl3
               Cl4     C8      C9      C10     C11     C12     C13     C14
               H8A     H8B     H8C     H11     H12     H13
PLAT300_ALERT_4_G Atom Site Occupancy of C38       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C55       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C69       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C70       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C54       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C67       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C68       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H38B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H39C      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H55C      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H69A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H69B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H70A      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H70B      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H70C      Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37C      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H37D      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H40A      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H40B      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41A      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41B      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41C      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53C      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H53D      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54A      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54B      Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H54C      Constrained at       0.25 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H66C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66D       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68C       Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       7.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       7.50 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H35A     ..H40A     .       1.51 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H34B     ..H41B     .       1.63 Ang.
                                                      x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H36B     ..H54C     .       2.01 Ang.
                                                   y,1/2-x,1+z  =      4_556 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H55B     ..H63C     .       1.59 Ang.
                                                  3/2-x,1/2-y,z  =      2_655 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H1A      ..H65A     .       2.05 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  S3       ..C41      .       3.29 Ang.
                                                    1/2-y,x,-1+z  =      3_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O29      ..C41      .       2.09 Ang.
                                                    1/2-y,x,-1+z  =      3_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C45      ..C40      .       3.11 Ang.
                                                    1/2-y,x,-1+z  =      3_554 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        170 A**3
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98020 Dev...       0.01 Ang.
             C54      -H54C            1_555   1_555 ........     #  272 Check
PLAT721_ALERT_1_G Bond    Calc     1.00000, Rep     0.98990 Dev...       0.01 Ang.
             C40      -H40A            1_555   1_555 ........     #  273 Check
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     0.99020 Dev...       0.01 Ang.
             C40      -H40B            1_555   1_555 ........     #  274 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.98010 Dev...       0.01 Ang.
             C41      -H41A            1_555   1_555 ........     #  276 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.73 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.86 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       535 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       593 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        65 Note
                  0  1  2,  -2  6  3,  -3  7  7,   1  5  1,   0  2  5,  -1  4  3,
                 -2 10  2,   1  1  3,  -1  5  1,   2  2  2,   5  5  1,  -2  5  2,
                  2  7  2,  -1  5  4,   1  2  1,   5  5  0,  -1  8  6,   1  3  1,
                  0  2  1,  -3  4  1,   0  4  0,  -1  6  1,   0  6  0,  -1  5  7,
                  4 11  2,  -5  6  5,   4  5  2,   3 14  1,   1  3  4,  -4  7  1,
                  0 12  2,   0  3  2,   0  0  6,   0  4  6,  -2  7  4,   8 13  2,
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```
                8  8  3,   2  4  1,  -8 35  8,   6  9  5,  -2  5  8,   5  7  1,
               -4 11  8,  -6  9  6,   4  4  2,  -3  9  1,   1  1  2,   1  5  2,
                2  3  6,   4 12  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.502 Note
              Predicted wR2: Based on SigI**2  5.38 or SHELX Weight 24.51
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 Cl-f'=    0.3292 Deviates from the B&C-Value     0.3281 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 Cl-f"=    0.5397 Deviates from the B&C-Value     0.5435 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
```

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

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

---

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@G7 - ellipsoid plot