checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G11

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@G11

Bond precision: C-C = 0.0125 A Wavelength=1.34050

Cell: a=29.9251(3) b=29.9251(3) c=19.4257(2)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17395.9(4)	17395.9(4)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 3(C7 H6 N2) [+ solvent]	C216 H364 Al32 N12 O110 Pb6 S12, 3(C7 H6 N2)
Sum formula	C237 H382 Al32 N18 O110 Pb6 S12 [+ solvent]	C237 H382 Al32 N18 O110 Pb6 S12
Mr	7734.91	7734.80
Dx,g cm-3	1.477	1.477
Z	2	2
Mu (mm-1)	5.109	5.253
F000	7820.0	7820.0
F000'	7799.39	
h,k,lmax	35,35,22	35,31,22
Nref	14826	14763
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)= 52.047

R(reflections)= 0.0675(11778)

wR2(reflections)= 0.1908(14763)

S = 1.024 Npar= 949

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 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.

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.77Ang From Pb2 2.73 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. 1.00Ang From Pb2 2.69 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_B Check Calcd Resid. Dens. 0.88Ang From Pb2 2.60 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 Pb3 1.62 eA-3

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

Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 1.34130-1.34150
           Wavelength given =    1.34050
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.73 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        5.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O17 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 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        C18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C43 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N4      0.119 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01246 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.136 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         60 Report
               -1  3  0,   1  3  0,   8  8  0,  -4 10  0,   0  2  1,   2  4  1,
               -1  6  1,   3  6  1,  -3  7  1,   6  7  1,  -9 11  1,  -6 11  1,
               -4 11  1,   6 15  1,  -6 17  1,   0  1  2,   1  1  2,   0  3  2,
                1  3  2,   3  4  2,   2  5  2,   3  5  2,  -5  6  2,  -5  7  2,
               -4  7  2,   1  7  2,   0  8  2,   1  9  2,   2 10  2,   5 10  2,
               10 10  2,  -4 11  2,   5 11  2,  -5 12  2,  -3  5  3,   2  5  3,
               -4  6  3,   2  6  3,  -1  7  3,   1 12  3,  -2  3  4,   4  4  4,
                1  5  4,   3  5  4,   2  7  4,   3  8  4,   2 14  4,  -3  9  5,
               -2 10  5,   7 12  5,   0  0  6,  -1  3  6,  -2  4  6,   2  4  6,
                1  8  6,   0  9  6,  -4 12  6,  -1  9  9,   1  3 10,  14 26 10,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.85Ang From Pb1              2.43 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.68Ang From Pb1              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.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From Pb2 2.37 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. 0.97Ang From Pb3 2.29 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. 0.82Ang From Pb2 2.21 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. 0.24Ang 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. 0.91Ang From Pb3 1.83 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

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         23 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          65 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          3 Report
              H10   H22   H4
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.73 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      11.31 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         20 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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              C39     C40     C55     C56     H39A    H39B    H39C    H40A
              H40B    H40C    H41A    H41B    H41C    H41D    H54A    H54B
              H54C    H54D    H55A    H55B    H55C    H56A    H56B    H56C
PLAT300_ALERT_4_G Atom Site Occupancy of N4         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N5         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 C58        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C59        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C60        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C61        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C62        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C63        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4         Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H58        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H61        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H62        Constrained at        0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H63        Constrained at        0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)          2% 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)       11.25 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H6A      ..H56C     .        1.95 Ang.
                                          y,1/2-x,-1+z  =      4_554 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         152 A**3
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         127 Do !
              O14 -AL5 -O12 -AL4    35.80  1.40   1_555   1_555   1_555   1_555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         128 Do !
              O14 -AL5 -O12 -AL8   -67.40  1.20   1_555   1_555   1_555   4_555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         177 Do !
              O12 -AL5 -O14 -PB2   165.30  1.00   1_555   1_555   1_555   1_555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         178 Do !
              O12 -AL5 -O14 -AL3   -88.90  1.10   1_555   1_555   1_555   1_555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         179 Do !
              O12 -AL5 -O14 -AL4    14.60  1.30   1_555   1_555   1_555   3_555
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .        1.14 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
              O23  -O23  -PB3     4_555   1_555   1_555 ......     #  224 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
```

```
             O23  -O23  -PB3     3_555   1_555   1_555 ......     #  225 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -PB3     2_555   1_555   1_555 ......     #  226 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     2_555   1_555   4_555 ......     #  227 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     4_555   1_555   1_555 ......     #  228 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     2_555   1_555   3_555 ......     #  229 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     4_555   1_555   3_555 ......     #  230 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     2_555   1_555   1_555 ......     #  231 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     4_555   1_555   2_555 ......     #  232 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     4_555   1_555   4_555 ......     #  233 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     3_555   1_555   2_555 ......     #  234 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     3_555   1_555   1_555 ......     #  235 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     2_555   1_555   2_555 ......     #  236 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     3_555   1_555   3_555 ......     #  237 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -AL7     3_555   1_555   4_555 ......     #  238 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -O23     3_555   1_555   2_555 ......     #  239 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -O23     4_555   1_555   2_555 ......     #  240 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O23  -O23  -O23     4_555   1_555   3_555 ......     #  241 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB1     4_555   1_555   1_555 ......     #  255 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB1     2_555   1_555   1_555 ......     #  256 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB1     3_555   1_555   1_555 ......     #  257 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     4_555   1_555   2_555 ......     #  258 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     2_555   1_555   3_555 ......     #  259 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     4_555   1_555   3_555 ......     #  260 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     3_555   1_555   2_555 ......     #  261 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     3_555   1_555   4_555 ......     #  262 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     2_555   1_555   2_555 ......     #  263 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     3_555   1_555   3_555 ......     #  264 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     4_555   1_555   1_555 ......     #  265 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL1     4_555   1_555   4_555 ......     #  266 Check
```

```
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL1     2_555   1_555   4_555 ......     #  267 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL1     2_555   1_555   1_555 ......     #  268 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL1     3_555   1_555   1_555 ......     #  269 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -O6      4_555   1_555   2_555 ......     #  270 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -O6      3_555   1_555   2_555 ......     #  271 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -O6      4_555   1_555   3_555 ......     #  272 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.13 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.79 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.82 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       455 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       61% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
               1  1  0,   0  0  1,   0  1  1,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
               1  1  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        57 Note
               0  1  2,  -2  3  4,   1  3  0,   2  6  3,   2  7  4,  -4 11  2,
              -1  7  3,  -4  7  2,   2 10  2,   3  5  4,   1  3 10,   1  3  2,
              -2 10  5,   2  4  6,  -5  7  2,  -6 17  1,   1  7  2,   3  5  2,
              -4 11  1,   5 11  2,  -1  3  6,   3  6  1,  -9 11  1,   1  1  2,
               7 12  5,   1  8  6,   0  0  6,  -6 11  1,   0  3  2,   1  9  2,
               3  4  2,   1  5  4,  -4  6  3,   2 14  4,   4  4  4,  -3  7  1,
              -4 12  6,   6  7  1,   6 15  1,   3  8  4,  -2  4  6,   0  8  2,
               8  8  0,   2  4  1,  -5 12  2,   0  9  6,  -3  9  5,  -3  5  3,
               2  5  2,  10 10  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.3 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ          4 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     2.440 Note
             Predicted wR2: Based on SigI**2  7.82 or SHELX Weight 18.63
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
```

---

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

```
  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  33 ALERT type 2 Indicator that the structure model may be wrong or deficient
  19 ALERT type 3 Indicator that the structure quality may be low
  65 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@G11 - ellipsoid plot