checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G13

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@G13

Bond precision: C-C = 0.0110 A Wavelength=1.34050

Cell: a=29.8451(2) b=29.8451(2) c=19.8380(2)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17670.3(3)	17670.3(3)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H368 Al32 N12 O110 Pb6 S12, 3(C12 H10 N2) [+ solvent]	C216 H368 Al32 N12 O110 Pb6 S12, 3(C12 H10 N2)
Sum formula	C252 H398 Al32 N18 O110 Pb6 S12 [+ solvent]	C252 H398 Al32 N18 O110 Pb6 S12
Mr	7931.19	7931.08
Dx,g cm-3	1.491	1.491
Z	2	2
Mu (mm-1)	5.040	5.181
F000	8032.0	8032.0
F000'	8011.76	
h,k,lmax	35,35,23	35,35,23
Nref	15072	15016
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)= 52.038

R(reflections)= 0.0567(13356)

wR2(reflections)= 0.1562(15016)

S = 1.028 Npar= 969

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 B

PLAT220_ALERT_2_B NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 7.7 Ratio

Author Response: These alerts are generated because there is a large amount of disorder in the structure. Some refined 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 assignment of atom types.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.93Ang From Pb1 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.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.93Ang From Pb2 2.89 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. 0.98Ang From Pb2 2.86 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. 0.96Ang From Pb1 2.77 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. 0.96Ang From Pb1 2.72 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. 0.89Ang From Pb2 2.66 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. 0.97Ang From Pb3 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.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.06Ang From Pb1 2.57 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.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.92Ang From Pb1 2.55 eA-3

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

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pb2 1.78 eA-3

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

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 ....       2.01 Report
PLAT213_ALERT_2_C Atom S2              has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom O20             has ADP max/min Ratio .....        3.4 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        5.7 Ratio
```

Author Response: These alerts are generated because there is a large amount of disorder in the structure. Some refined 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 assignment of atom types.

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  S   Ueq(max)/Ueq(min) Range        3.2 Ratio
```

Author Response: These alerts are generated because there is a large amount of disorder in the structure. Some refined 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 assignment of atom types.

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        8.9 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C5 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         C4 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
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01102 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H7       ..H19      .       1.91 Ang.
                                                y,1/2-x,z  =      4_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3       --H3       .     Please Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.467 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         55 Report
                2  2  0,  -1  5  0,   0  6  0,   2  6  0,   1  1  1,  -1  2  1,
                1  3  1,  -1  5  1,   0  5  1,   5  6  1,   3  7  1, -10 13  1,
                3 17  1,   0  1  2,   0  3  2,   1  3  2,   1  4  2,  -3  5  2,
               -2  5  2,  -1  5  2,   3  5  2,  -4  6  2,   0  6  2,   5  7  2,
                7  7  2,   0  8  2,  -1  9  2,  -5 11  2,   4 11  2,   7 15  2,
                0  2  3,  -2  3  3,  -2  6  3,   2  3  4,   3  4  4,  -3  5  4,
               -7 10  4,  -5 10  4,  -5 11  4,   4  6  6,  -1 10  7,   2 15 10,
                1 15 11,   2 15 11,   1 16 12,   2 16 12,   1 16 13,   2 16 13,
                1 16 14,   2 16 14,   1 16 15,   2 16 15,   1 16 16,   2 16 16,
                2 15 19,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From Pb1             2.44 eA-3
```

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

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From Pb3            1.88 eA-3
```

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

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PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Pb3            1.81 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.

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PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Pb2           -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82Ang From Pb3           -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From Pb1           -1.62 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From Pb1           -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.89Ang From Pb1           -1.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3       .      -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7       .      -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23      .      -0.32 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         22 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 ..............          3 Report
               H3    H7    H23
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.72 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      49.57 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         19 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
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
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             C56     C57     H54A    H54B    H54C    H54D    H56A    H56B
             H56C    H57A    H57B    H57C
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 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 C64        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C65        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C66        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C67        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C68        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 H58        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59        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
PLAT300_ALERT_4_G Atom Site Occupancy of H64        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H66        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H69        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
PLAT411_ALERT_2_G Short Inter H...H Contact  H32      ..H67      .       1.98 Ang.
                                            -1/2+y,1-x,1-z  =      7_566 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H50B     ..H56B     .       2.13 Ang.
                                            1-y,-1/2+x,1-z  =      8_656 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H3       ..H54A     .       2.09 Ang.
                                                     x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H3       ..H56A     .       1.95 Ang.
                                                     x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         73 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB2     3_555   1_555   1_555 ......     #  195 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB2     4_555   1_555   1_555 ......     #  196 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -PB2     2_555   1_555   1_555 ......     #  197 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     2_555   1_555   2_555 ......     #  198 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     3_555   1_555   1_555 ......     #  199 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     3_555   1_555   3_555 ......     #  200 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     2_555   1_555   1_555 ......     #  201 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     4_555   1_555   1_555 ......     #  202 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     3_555   1_555   2_555 ......     #  203 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O6   -O6   -AL4     4_555   1_555   4_555 ......     #  204 Check
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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL4     4_555   1_555   3_555 ......     #  205 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL4     3_555   1_555   4_555 ......     #  206 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL4     2_555   1_555   3_555 ......     #  207 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL4     2_555   1_555   4_555 ......     #  208 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O6   -O6   -AL4     4_555   1_555   2_555 ......     #  209 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 ......     #  210 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 ......     #  211 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 ......     #  212 Check
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SpGr)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.79 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.73 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.81 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       343 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       78% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
                1  1  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        37 Note
                1  4  2,   0  1  2,  -3  5  4,   2  3  4,  -2  6  3,   5  6  1,
                7  7  2,  -1  5  1,   2  2  0,  -2  3  3,   0  5  1,   3  5  2,
                0  8  2,   0  6  2,   2  6  0, -10 13  1,   4 11  2,   3 17  1,
                5  7  2,  -5 11  2,  -7 10  4,  -1  5  0,   1  3  1,   7 15  2,
               -1  9  2,   3  7  1,  -5 11  4,   4  6  6,   3  4  4,   0  2  3,
                0  3  2,  -1  2  1,  -2  5  2,   1  3  2,   0  6  0,  -5 10  4,
               -1  5  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     3.392 Note
              Predicted wR2: Based on SigI**2  4.60 or SHELX Weight 15.19
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
PLAT984_ALERT_1_G The  C-f'=    0.0150 Deviates from the B&C-Value     0.0137 Check
PLAT984_ALERT_1_G The Al-f'=    0.1760 Deviates from the B&C-Value     0.1771 Check
PLAT984_ALERT_1_G The  O-f'=    0.0410 Deviates from the B&C-Value     0.0389 Check
PLAT984_ALERT_1_G The Pb-f'=   -4.2650 Deviates from the B&C-Value    -4.4950 Check
PLAT985_ALERT_1_G The Al-f"=    0.1840 Deviates from the B&C-Value     0.1873 Check
PLAT985_ALERT_1_G The Pb-f"=    7.1980 Deviates from the B&C-Value     6.8412 Check
PLAT985_ALERT_1_G The  S-f"=    0.4240 Deviates from the B&C-Value     0.4295 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
11 **ALERT level B** = A potentially serious problem, consider carefully
31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
93 **ALERT level G** = General information/check it is not something unexpected

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  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  44 ALERT type 2 Indicator that the structure model may be wrong or deficient
  18 ALERT type 3 Indicator that the structure quality may be low
  52 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.
```

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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
```

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@G13 - ellipsoid plot