checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G12

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@G12

Bond precision: C-C = 0.0121 A Wavelength=1.34050

Cell: a=29.9771(3) b=29.9771(3) c=19.4854(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17510.1(4)	17510.1(4)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H360 Al32 N12 O110 Pb6 S12, 3(C10 H8 N2) [+ solvent]	C216 H360 Al32 N12 O110 Pb6 S12, 3(C10 H8 N2)
Sum formula	C246 H384 Al32 N18 O110 Pb6 S12 [+ solvent]	C246 H384 Al32 N18 O110 Pb6 S12
Mr	7845.01	7844.91
Dx,g cm-3	1.488	1.488
Z	2	2
Mu (mm-1)	5.082	5.225
F000	7932.0	7932.0
F000'	7911.62	
h,k,lmax	35,35,22	32,35,22
Nref	14929	14897
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 0.998 Theta(max)= 52.048

R(reflections)= 0.0582(12193)

wR2(reflections)= 0.1635(14897)

S = 1.038 Npar= 967

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C24 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.

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 .... 2.58 Report
PLAT213_ALERT_2_C Atom O24 has ADP max/min Ratio ..... 3.5 prolat
PLAT215_ALERT_3_C Disordered C54 has ADP max/min Ratio ..... 3.9 Note
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.9 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C40 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C51 Check
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 S3 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 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_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 N6 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 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.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 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        C27 Check
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Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
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Author Response: These alerts are generated because of a slight unresolved disorder caused by free rotation of the flexible chain at the end of the ligand.Some refi commands such as DELU, SIMU and ISOR were used to address such abnormal Ueq value, but failed. After inspection, this does not affect the correct assign of atom types.

```
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    2)        2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1       0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N4       0.114 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01215 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C15      - C17      .       1.43 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.626 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         30 Report
               -1  3  0,  -2  4  1,  -4  5  1,   4  6  1,   3 17  1,   0  1  2,
                1  2  2,   0  3  2,  -2  5  2,   3  5  2,   5  7  2,  -1  9  2,
               -2 10  2,   3 10  2,  -5 11  2,   0  2  3,   6 10  3,  -7 12  3,
                2  5  4,  -2  7  4,  -2 14  4,  -2  4  6,  -9 11  6,   0 12  6,
               -4 14  6,   3 11 18,   3 12 18,   3 13 21,   4 13 21,   5 13 21,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.30Ang From Pb1             2.22 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.05Ang From Pb2             2.16 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From Pb2             1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From Pb1             1.88 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Pb3             1.81 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.89Ang From O19             1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.24Ang From Pb1             1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.11Ang From O2              1.73 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Pb3             1.68 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From Pb2             1.53 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Pb2       1.39 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Pb3       1.30 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         21 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          20 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............           2 Report
               H3    H21
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      28.55 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         15 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
              C53     C54     H53A    H53B    H53C    H54A    H54B    H54C
PLAT300_ALERT_4_G Atom Site Occupancy of C7         Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7B        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7C        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6C        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42A       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42B       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H42C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52C       Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H52D       Constrained at       0.25 Check
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 H58        Constrained at       0.75 Check
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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 H65        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
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H53C     ..H57C     .       1.73 Ang.
                                             -1/2+y,1-x,1-z  =      7_566 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         72 A**3
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             H42A    -C42     -H42B       1_555  1_555  1_555     #  581 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -PB1      4_565   1_555   1_555 ......     #  182 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -PB1      3_655   1_555   1_555 ......     #  183 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -PB1      2_665   1_555   1_555 ......     #  184 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      3_655   1_555   4_565 ......     #  185 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      3_655   1_555   3_655 ......     #  186 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      4_565   1_555   3_655 ......     #  187 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      2_665   1_555   3_655 ......     #  188 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      4_565   1_555   1_555 ......     #  189 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      2_665   1_555   4_565 ......     #  190 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      4_565   1_555   2_665 ......     #  191 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      4_565   1_555   4_565 ......     #  192 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      3_655   1_555   2_665 ......     #  193 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      3_655   1_555   1_555 ......     #  194 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      2_665   1_555   1_555 ......     #  195 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -AL1      2_665   1_555   2_665 ......     #  196 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -O2       3_655   1_555   2_665 ......     #  197 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -O2       4_565   1_555   3_655 ......     #  198 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O2   -O2   -O2       4_565   1_555   2_665 ......     #  199 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.01 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.81 Info
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PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.83 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        127 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         57% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                  1  1  0,   0  0  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         23 Note
                 -1  3  0,   0  3  2,   0  1  2,  -2 10  2,   1  2  2,   3  5  2,
                 -2  7  4,  -5 11  2,  -2  5  2,   0  2  3,  -2  4  1,  -1  9  2,
                  2  5  4,  -9 11  6,   3 17  1,  -2  4  6,  -7 12  3,  -4  5  1,
                  0 12  6,  -4 14  6,   5  7  2,   3 10  2,  -2 14  4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.4 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           3 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.449 Note
              Predicted wR2: Based on SigI**2  4.74 or SHELX Weight 15.76
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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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  38 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 112 ALERT level G = General information/check it is not something unexpected

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  38 ALERT type 2 Indicator that the structure model may be wrong or deficient
  20 ALERT type 3 Indicator that the structure quality may be low
  70 ALERT type 4 Improvement, methodology, query or suggestion
  11 ALERT type 5 Informative message, check
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checkCIF publication errors

Alert level A

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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).
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PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
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   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
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Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```

```
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

Datablock SAlOC-1@G12 - ellipsoid plot