checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G6

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@G6

Bond precision: C-C = 0.0155 A Wavelength=1.34050

Cell: a=30.0301(3) b=30.0301(3) c=19.2959(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17401.2(5)	17401.2(5)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H358 Al32 N12 O110 Pb6 S12, 3(C9 H12) [+ solvent]	C216 H358 Al32 N12 O110 Pb6 S12, 3(C9 H12)
Sum formula	C243 H394 Al32 N12 O110 Pb6 S12 [+ solvent]	C243 H394 Al32 N12 O110 Pb6 S12
Mr	7735.00	7734.90
Dx,g cm-3	1.476	1.476
Z	2	2
Mu (mm-1)	5.104	5.248
F000	7832.0	7832.0
F000'	7811.32	
h,k,lmax	35,35,22	34,35,22
Nref	14850	14796
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)= 0.0635(10743)

wR2(reflections)= 0.2018(14796)

S = 1.046 Npar= 934

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 2.01 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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.2 Ratio

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3 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.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pb2 1.96 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 ....       2.82 Report
PLAT213_ALERT_2_C Atom O1              has ADP max/min Ratio .....        3.3 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        4.9 Ratio
```

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.

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        8.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C8 Check
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C43 Check
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C45 Check
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C50 Check
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C51 Check
```

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C55 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        S1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O28 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        N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C7 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       C44 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    2)       2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1     0.117 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C57     0.229 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....          C49 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds .............   0.01545 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C55      - C56      .      1.69 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H2A      ..H3B      .      1.93 Ang.
                                             x,y,z  =      1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H6B      ..H53A     .      2.01 Ang.
                                          1-x,2-y,1-z  =      5_676 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         52 Report
                1  3  0,   4  4  0,  -1  7  0,  -3  4  1,  -2  4  1,   4  4  1,
                1  5  1,   2  5  1,   3  5  1,   5  5  1,   2  7  1,   3  7  1,
                6  8  1,   0  9  1,   3  9  1,   0  0  2,   0  1  2,  -1  2  2,
               -1  5  2,   2  5  2,  -2  7  2,   7  7  2,  -4 11  2,   1  1  3,
                1  4  3,   2  4  3,   1  7  3,   3  8  3,   1 11  3,   5  8  4,
                7 10  5,   4 11  5,  -2 13  5,  15 28  5,  -1  3  6,   4  4  6,
               -4  7  6,   1  8  6,   5  9  6,   2 10  6,   5 13  6,  -1  8  7,
```

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              2  5  8, -14 22 14, -13 22 14, -12 22 14, -14 23 14, -14 22 15,
            -13 22 15,   3 19 18,   3 20 18,   4 20 18,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.85Ang From Pb2            2.23 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.96Ang From Pb2            1.95 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Pb1            1.76 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.64Ang From Pb1            1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From Pb2            1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From Pb3            1.61 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.16Ang From Pb1            1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.84Ang From Pb3            1.59 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From O24     .      0.91 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.04Ang From O21     .     -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2B       .     -0.31 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        30 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         25 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
            H8    H29
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      2.74 %
PLAT069_ALERT_1_G Atom Label Without Numerical Part ..............        Al Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.14 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        24 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par    0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar    0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0200 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C47        Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C48        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47A       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47B       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47C       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H48A       Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H48B       Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H48C       Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49A       Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49B       Constrained at      0.25 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 C64        Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C65        Constrained at      0.75 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H57A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H57C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H58A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H58B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H58C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59A       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59B       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H59C       Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H60        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 H64        Constrained at       0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)         1% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)     15.75 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C49      - C50      .       1.54 Ang.
PLAT411_ALERT_2_G Short Inter H...H Contact  H3A      ..H64      .       2.10 Ang.
                                                    x,y,1+z  =      1_556 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H3A      ..H58B     .       2.00 Ang.
                                                    x,y,1+z  =      1_556 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H3B      ..H58B     .       1.20 Ang.
                                                    x,y,1+z  =      1_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C3       ..C58      .       2.84 Ang.
                                                    x,y,1+z  =      1_556 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        405 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2 Note
             Al00    Al0B
PLAT721_ALERT_1_G Bond    Calc     0.99000, Rep     0.97990 Dev...       0.01 Ang.
             C48      -H48C            1_555   1_555 ........     #  247 Check
PLAT722_ALERT_1_G Angle   Calc      104.00, Rep      105.10 Dev...       1.10 Degree
             H2A     -C2      -H2B        1_555  1_555  1_555     #  542 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      111.80 Dev...       1.20 Degree
             C49     -C48     -H48B       1_555  1_555  1_555     #  544 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)       .       2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)       .       2.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al        (III)      .       2.77 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al00      (III)      .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)      .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al0B      (III)      .       2.73 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)      .       2.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)      .       2.87 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        328 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         41% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               1  1  0,   0  0  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         42 Note
              -1  2  2,   0  0  2,   1  3  0,   0  1  2,   1  5  1,  -4  7  6,
               4 11  5,   2  5  2,   5  9  6,  -4 11  2,   1  4  3,   1  8  6,
               6  8  1,   7  7  2,  -2  7  2,   5  5  1,   2  7  1,   3  8  3,
               0  9  1,  -1  3  6,  -1  5  2,  -2  4  1,   4  4  1,   4  4  0,
               1 11  3,   2  5  8,   7 10  5,  -2 13  5,   4  4  6,   2  4  3,
               5  8  4,  -3  4  1,   3  9  1,   3  7  1,   2 10  6,   1  1  3,
               1  7  3,   5 13  6,   3  5  1,  -1  8  7,   2  5  1,  -1  7  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........         3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.407 Note
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             Predicted wR2: Based on SigI**2  4.58 or SHELX Weight 19.30
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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```
   1 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  43 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  88 ALERT level G = General information/check it is not something unexpected

  14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  51 ALERT type 2 Indicator that the structure model may be wrong or deficient
  15 ALERT type 3 Indicator that the structure quality may be low
  45 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@G6 - ellipsoid plot