checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G14

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@G14

Bond precision: C-C = 0.0146 A Wavelength=1.34050

Cell: a=30.0170(3) b=30.0170(3) c=19.5023(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	17572.0(5)	17572.0(5)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C216 H364 Al32 N12 O110 Pb6 S12, 2(C8 H10 N), 2(C5 H4 N) [+ sol	C216 H364 Al32 N12 O110 Pb6 S12, 0.5(C52 H56 N8)
Sum formula	C242 H392 Al32 N16 O110 Pb6 S12 [+ solvent]	C242 H392 Al32 N16 O110 Pb6 S12
Mr	7777.02	7776.91
Dx,g cm-3	1.470	1.470
Z	2	2
Mu (mm-1)	5.059	5.201
F000	7872.0	7872.0
F000'	7851.44	
h,k,lmax	38,38,25	38,31,25
Nref	19898	19373
Tmin,Tmax	0.563,0.771	0.248,1.000
Tmin'	0.337	

Correction method= # Reported T Limits: Tmin=0.248 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 60.036

R(reflections)= 0.0701(13018) wR2(reflections)= 0.2239(19373)

S = 1.047 Npar= 977

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 2.32 eA-3

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

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb2 2.07 eA-3

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

Alert level B

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N3 Check

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.

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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.17 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.4 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 O24 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C39 Check

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C57 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C59 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C31 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C43 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C49 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C51 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C56 Check
```

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.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C66 Check
```

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.

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.125 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N5      0.150 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N4      0.150 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for .....          C6 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0146 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H18B     ..H63A     .       2.10 Ang.
                                              1-x,2-y,1-z  =      5_676 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.918 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         73 Report
                1  3  0,   0  4  0,  -3  5  0,   1  5  0,   0  6  0,   2  6  0,
                8  8  0,   5  9  0,   6 10  0, -21 29  0, -19 29  0, -17 29  0,
                1  1  1,  -2  3  1,  -1  3  1,  -2  4  1,  -4  5  1,  -2  5  1,
                0  5  1,  -3  7  1,   2  9  1,  -8 10  1,   3 10  1,   2 11  1,
              -21 29  1, -20 29  1,   0  0  2,   0  3  2,   1  3  2,  -2  4  2,
                3  4  2,   4  5  2,   6  6  2,  -4  7  2,   1  9  2,  -9 10  2,
                5 10  2,  -6 12  2,   0 12  2,   0  2  3,   1  3  3,   1  5  3,
                2  6  3,  -1  7  3,   7 12  3,  -3  4  4,  -2  5  4,   2  5  4,
               -1  6  4,   2  6  4,  -2 12  4,   2 14  4,  -1  4  5,   3  4  5,
               -3  6  5,   5  9  5,  -5  8  6,   1  8  6,   1  9  6,  -4 16  6,
                0  0  7,   3  3  7,   3  7  7,   0  8  7,   5 13  7,   4  4  9,
               -1 12  9,   0  0 14,  15 21 14,  15 22 14,  14 24 14,  14 25 14,
                1 17 18,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From Pb2             2.19 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.59Ang From Pb1             1.97 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Pb2             1.56 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From O5      .       0.70 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17C      .      -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         28 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          45 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
              H12   H27
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C216 H364 Al32 N12 O110 Pb6 S12, 2(C8 H10 N), 2(C5 H4 N)
              Rep.: C216 H364 Al32 N12 O110 Pb6 S12, 0.5(C52 H56 N
```

8)

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 0.14 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 23 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 5 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR 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
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
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

C41	C42	H40A	H40B	H40C	H40D	H41A	H41B
H41C	H42A	H42B	H42C	N5	C6	C7	C8
C9	C10	C11	C12	C13	H6A	H6B	H7A
H7B	H8A	H8B	H9	H10	H12A	H13	N4
C1	C2	C3	C4	C5	H1	H2	H4
H5							

PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 1% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2) 9.50 Check
PLAT411_ALERT_2_G Short Inter H...H Contact H7B ..H62A . 2.08 Ang.
1-x,2-y,1-z = 5_676 Check
PLAT411_ALERT_2_G Short Inter H...H Contact H1 ..H57 . 2.11 Ang.
x,y,z = 1_555 Check
PLAT411_ALERT_2_G Short Inter H...H Contact H1 ..H47 . 2.14 Ang.
y,3/2-x,z = 4_565 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H37B ..H41A . 1.99 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H39B ..H42B . 2.12 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H42C ..H61B . 2.10 Ang.
-1+y,3/2-x,z = 4_465 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C2 ..C6 . 2.53 Ang.
2-y,1/2+x,1-z = 8_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 ..C6 . 1.48 Ang.
2-y,1/2+x,1-z = 8_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 ..C7 . 2.69 Ang.
2-y,1/2+x,1-z = 8_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C3 ..C8 . 3.10 Ang.
2-y,1/2+x,1-z = 8_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C4 ..C6 . 2.42 Ang.
2-y,1/2+x,1-z = 8_766 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 109 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 0.00 Deg.
O10 -O10 -PB1 3_655 1_555 1_555 ..... # 185 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 0.00 Deg.
O10 -O10 -PB1 4_565 1_555 1_555 ..... # 186 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 0.00 Deg.
O10 -O10 -PB1 2_665 1_555 1_555 ..... # 187 Check

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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     2_665   1_555   4_565 ......     #  188 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     2_665   1_555   2_665 ......     #  189 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     3_655   1_555   2_665 ......     #  190 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     4_565   1_555   1_555 ......     #  191 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     4_565   1_555   3_655 ......     #  192 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     3_655   1_555   4_565 ......     #  193 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     3_655   1_555   1_555 ......     #  194 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     2_665   1_555   3_655 ......     #  195 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     2_665   1_555   1_555 ......     #  196 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     4_565   1_555   2_665 ......     #  197 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     4_565   1_555   4_565 ......     #  198 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -AL2     3_655   1_555   3_655 ......     #  199 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -O10     4_565   1_555   3_655 ......     #  200 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -O10     3_655   1_555   2_665 ......     #  201 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              O10  -O10  -O10     4_565   1_555   2_665 ......     #  202 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al4       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.75 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.79 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.84 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       436 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 !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
                1  1  0,   0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       446 Note
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        65 Note
              -23 26  9,  18 19 17,   0  2  3,   0  4  0,   1  1  1,   2  6  3,
                1  8  6,  -1  3  1,   1  3  2,   0  5  1,  -2 12  4,   4  4  9,
               -9 25 18,  -3  7  1,   0 12  2,   5  9  5,   7 12  3,   2  5  4,
               -3  4  4,   2 14  4,   1  9  2,  -2  4  2,   2 11  1,  -4  7  2,
                3  3  7,  15 25 14,   3  4  2,  -1  4  5,   3  7  7,   0  3  2,
               -4  5  1,   1  5  3,  -5 26 18,   2  9  1,   5 13  7,  -2  5  1,
                2  6  0,  -9 10  2,  -1  6  4,  -2  5  4,   1  3  3,  -3  5  0,
               -6 12  2,   1  9  6,   4  5  2,  -3  6  5,   6  6  2,  -5  8  6,
                0  8  7,  -8 10  1,
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PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....        3.0 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ          7 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      3.728 Note
             Predicted wR2: Based on SigI**2  6.01 or SHELX Weight 21.38
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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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2 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
35 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
83 **ALERT level G** = General information/check it is not something unexpected

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
48 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
30 ALERT type 4 Improvement, methodology, query or suggestion
12 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).
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
```

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Datablock SAlOC-1@G14 - ellipsoid plot