# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAlOC-1@G5

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@G5

---

Bond precision: C-C = 0.0177 A Wavelength=1.34050

Cell: a=30.0020(4) b=30.0020(4) c=19.4409(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 17499.2(6) | 17499.1(6) |
| Space group | P 4/n | P 4/n |
| Hall group | -P 4a | -P 4a |
| Moiety formula | C216 H360 Al32 N12 O110 Pb6 S12, 2(C6 H6) [+ solvent] | C216 H360 Al32 N12 O110 Pb6 S12, 2(C6 H6) |
| Sum formula | C228 H372 Al32 N12 O110 Pb6 S12 [+ solvent] | C228 H372 Al32 N12 O110 Pb6 S12 |
| Mr | 7532.68 | 7532.57 |
| Dx,g cm-3 | 1.430 | 1.430 |
| Z | 2 | 2 |
| Mu (mm-1) | 5.066 | 5.208 |
| F000 | 7608.0 | 7608.0 |
| F000' | 7586.96 | |
| h,k,lmax | 35,35,22 | 35,33,22 |
| Nref | 14924 | 14877 |
| Tmin,Tmax | | 1.000,1.000 |
| Tmin' | | |

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

Data completeness= 0.997 Theta(max)= 52.046

R(reflections)= 0.0785( 10320)

wR2(reflections)= 0.2421( 14877)

S = 1.027 Npar= 928

---

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**

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.86Ang From Pb1 4.59 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_A Check Calcd Resid. Dens. 1.11Ang From Pb2 3.98 eA-3

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.96Ang From Pb1 3.85 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_A Check Calcd Resid. Dens. 1.08Ang From Pb3 3.77 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_A Check Calcd Resid. Dens. 0.85Ang From Pb2 3.57 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.**

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Pb1 3.49 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 Pb3 2.09 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**

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 4.83 Report

**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. 1.05Ang From Pb3 3.36 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. 0.23Ang From Pb2 2.85 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

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C33 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C36 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C53 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C56 Check
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         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 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        C40 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C50 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.127 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C11      0.129 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01767 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C4       - C5       .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C22      - C23      .       1.43 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H4A      ..H5B      .       1.95 Ang.
                                                     x,y,z  =      1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H35A     ..H49      .       2.11 Ang.
                                                -x,1-y,1-z  =      5_566 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -2.471 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         45 Report
               -1  3  0,   0  4  0,   2  6  0,   0  8  0,   2 10  0,   1  1  1,
                1  3  1,   0  4  1,   7  7  1,  -3  9  1, -10 13  1,   1  1  2,
               -3  4  2,   1  4  2,  -3  6  2,  -1  7  2,   4  7  2,   1  8  2,
               -2 10  2,   9 10  2,  -5 11  2,   2  2  3,  -1  4  3,  -2  5  3,
                2 12  3,   2 14  3,   1  3  4,   2  5  4,   5  7  4,   6  8  4,
                2 12  4,  -1  3  5,  -1  3  6,  -2  4  6,  -1  8  6,  -4  5  8,
               14 27 10, -17 20 14, -16 20 14, -18 21 14, -17 21 14, -16 21 14,
              -17 22 14, -16 22 14,  -3 21 17,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.77Ang From Pb1             2.09 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From Pb2             2.05 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Pb2             1.95 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Pb3            1.94 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.88Ang From Pb2            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.**

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Pb2            1.74 eA-3
```

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

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.88Ang From Pb2            1.73 eA-3
```

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

```
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O7      .       0.95 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6A       .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H25C      .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H44A      .      -0.40 eA-3
```

---

**Alert level G**

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         26 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          66 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          2 Report
               H10   H23
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       0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.65 Why ?
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          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
               C9      C10     C24     C25     C38     C39     H8A     H8B
               H9A     H9B     H9C     H10A    H10B    H10C    H22     H22A
               H24A    H24B    H24C    H25A    H25B    H25C    H37A    H37B
               H37C    H37D    H38A    H38B    H38C    H39A    H39B    H39C
               C11     C59     C60     C61     C62     C87     H11     H59
               H60     H61     H62     H87
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)          3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)        100% Note
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for          C4 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C56 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H5A      ..H10A     .        1.79 Ang.
                                                    x,y,z  =       1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H22A     ..H23C     .        2.09 Ang.
                                                    x,y,z  =       1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H38C     ..H55A     .        1.66 Ang.
                                                 1/2-y,1+x,z  =       3_565 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........           ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -PB1     3_555   1_555   1_555 ......     #  190 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -PB1     2_555   1_555   1_555 ......     #  191 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -PB1     4_555   1_555   1_555 ......     #  192 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     3_555   1_555   3_555 ......     #  193 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     3_555   1_555   1_555 ......     #  194 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     2_555   1_555   2_555 ......     #  195 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     2_555   1_555   3_555 ......     #  196 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     4_555   1_555   3_555 ......     #  197 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     4_555   1_555   2_555 ......     #  198 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     4_555   1_555   1_555 ......     #  199 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     4_555   1_555   4_555 ......     #  200 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
               O7   -O7   -AL1     2_555   1_555   1_555 ......     #  201 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...        0.00 Deg.
```

```
             O7   -O7   -AL1     3_555   1_555   4_555 ......     #  202 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O7   -O7   -AL1     2_555   1_555   4_555 ......     #  203 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O7   -O7   -AL1     3_555   1_555   2_555 ......     #  204 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O7   -O7   -O7      3_555   1_555   2_555 ......     #  205 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O7   -O7   -O7      4_555   1_555   3_555 ......     #  206 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
             O7   -O7   -O7      4_555   1_555   2_555 ......     #  207 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C6 H6
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.06 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 Al6       (III)     .       2.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al7       (III)     .       2.83 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al8       (III)     .       2.73 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       581 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       34% 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        33 Note
               1  3  1,  -2 10  2,   0  8  0,  -1  7  2,   2  6  0,   2 14  3,
              -1  3  5,  -1  3  6,   2 12  3, -10 13  1,  -1  4  3,   1  4  2,
               0  4  0,   4  7  2,  -2  5  3,  -3  6  2,  -1  8  6,  -3  9  1,
               1  8  2,   0  4  1,   2 12  4,  -5 11  2,  -3  4  2,   2 10  0,
              -4  5  8,   7  7  1,  -2  4  6,   2  5  4,   5  7  4,   6  8  4,
               1  3  4,   2  2  3,   9 10  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.4 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ         2 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     4.615 Note
             Predicted wR2: Based on SigI**2  5.25 or SHELX Weight 23.58
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
```

---

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
53 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
27 ALERT type 4 Improvement, methodology, query or suggestion
10 ALERT type 5 Informative message, check

# checkCIF publication errors

**Alert level A**

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

### Publication of your CIF

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

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

### Validation response form

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

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
```

```
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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

---

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

**Datablock SAlOC-1@G5** - ellipsoid plot