

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SAIOC-1@G9

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: SAIOC-1@G9

| | | | |
|------------------------|--|---|---------------------------|
| Bond precision: | C-C = 0.0125 Å | Wavelength=1.34050 | |
| Cell: | a=30.3099 (3) alpha=90 | b=30.3099 (3) beta=90 | c=19.6250 (3) gamma=90 |
| Temperature: | 100 K | | |
| | Calculated | Reported | |
| Volume | 18029.3 (4) | 18029.3 (5) | |
| Space group | P 4/n | P 4/n | |
| Hall group | -P 4a | -P 4a | |
| Moiety formula | C216 H362 Al32 N12 O110 Pb6 S12, 3(C12 H17 B O2) [+ solvent] | C216 H362 Al32 N12 O110 Pb6 S12, 3(C12 H17 B O2) | |
| Sum formula | C252 H413 Al32 B3 N12 O116 Pb6 S12 [+ solvent] | C252 H413 Al32 B3 N12 O116 Pb6 S12 | |
| Mr | 7990.68 | 7990.57 | |
| Dx, g cm ⁻³ | 1.472 | 1.472 | |
| Z | 2 | 2 | |
| Mu (mm ⁻¹) | 4.946 | 5.085 | |
| F000 | 8104.0 | 8104.0 | |
| F000' | 8084.02 | | |
| h, k, lmax | 39, 39, 25 | 39, 39, 25 | |
| Nref | 20531 | 19912 | |
| Tmin, Tmax | | 1.000, 1.000 | |
| Tmin' | | | |

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

Data completeness= 0.970 Theta (max) = 60.200

R(reflections)= 0.0664(14319)

wR2 (reflections)=
0.1980(19912)

S = 1.067

Npar= 1004

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. 0.87Ang From Pb01

4.48 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 Pb02

4.23 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. 0.90Ang From Pb03

4.08 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. 0.99Ang From Pb02

4.01 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.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.00Ang From Pb01

3.65 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 Pb02 2.49 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 Pb01 2.41 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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.95Ang From Pb03 2.81 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.

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Pb03 1.77 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.

🟡 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 | 2.94 Report |
| PLAT213_ALERT_2_C | Atom O8 has ADP max/min Ratio | 3.3 prolat |
| 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 | 5.6 Ratio |
| PLAT222_ALERT_3_C | NonSolvent Resd 1 H Uiso(max) / Uiso(min) Range | 6.0 Ratio |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C02H Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | S00D Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | S01Z Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | N01C Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | N01S Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C016 Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C01B Check |

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PLAT242_ALERT_2_C Low      'MainMol' Ueq as Compared to Neighbors of      C01I Check
PLAT242_ALERT_2_C Low      'MainMol' Ueq as Compared to Neighbors of      C025 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      001V      0.113 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....      0.01249 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C028      - C02J      .      1.42 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C18       - C02H      .      1.65 Ang.
PLAT414_ALERT_2_C Short  Intra D-H...H-X      H00M      ..H016      .      1.99 Ang.

3/2-y,x,z = 3_655 Check

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4      Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600      78 Report
      0 2 0, 2 2 0, -1 3 0, 3 3 0, -6 8 0, 22 28 0,
      21 29 0, 20 30 0, 5 35 0, 4 36 0, -3 4 1, 0 4 1,
      1 6 1, -6 7 1, 0 9 1, 9 11 1, 21 29 1, 0 0 2,
      0 1 2, 0 3 2, 1 3 2, 2 4 2, 4 4 2, -2 5 2,
      -3 6 2, -1 7 2, 0 8 2, -6 9 2, -5 9 2, -1 9 2,
      6 9 2, -2 10 2, 0 2 3, 2 2 3, -2 5 3, -6 7 3,
      -5 7 3, 7 35 3, 8 35 3, 3 3 4, 1 6 4, -2 7 4,
      0 11 4, 8 34 4, 9 34 4, 10 34 4, 1 2 5, 2 7 5,
      3 7 5, 9 32 5, 10 32 5, 11 32 5, 9 33 5, 10 33 5,
      9 34 5, -3 8 6, -1 8 6, 4 9 6, 6 9 6, 9 12 6,
      -3 13 6, 1 14 6, 0 15 6, 10 30 6, 11 30 6, 10 31 6,
      -5 11 7, -4 5 8, -15 26 11, -14 26 13, -12 24 15, -12 25 15,
      -11 24 16, -8 12 20, -7 12 20, -9 11 21, -8 11 21, -8 12 21,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From Pb02      2.16 eA-3

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

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PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From Pb01      2.11 eA-3
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Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.11Ang From Pb01      2.05 eA-3
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Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

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PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.12Ang From Pb03      1.96 eA-3
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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. 1.00Ang From Pb01 1.93 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. 1.12Ang From Pb01 1.63 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. 1.04Ang From O00 . | 0.96 eA-3 |
| PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From O010 . | -0.47 eA-3 |
| PLAT977_ALERT_2_C Check Negative Difference Density on H16D . | -0.32 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 | 2 Note | |
| PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms | 69 Report | |
| PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms H00M H00W | 2 Report | |
| PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . | 2.73 % | |
| PLAT069_ALERT_1_G Atom Label Without Numerical Part | H Do ! | |
| PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large | 0.12 Report | |
| PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX 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 | 2 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 | |
| PLAT299_ALERT_4_G Atom Site Occupancy Constrained at | 0.5 Check | |
| C1 C27 C30 C31 H1A H1B H1C | H6 | |
| H16A H16B H16C H16D H27A H27B H27C | | H30A |
| H30B H30C H31A H31B H31C Hs Ht | | |
| PLAT300_ALERT_4_G Atom Site Occupancy of O01V Constrained at | 0.75 Check | |
| PLAT300_ALERT_4_G Atom Site Occupancy of O01X Constrained at | 0.75 Check | |
| PLAT300_ALERT_4_G Atom Site Occupancy of C22 Constrained at | 0.75 Check | |
| PLAT300_ALERT_4_G Atom Site Occupancy of C28 Constrained at | 0.75 Check | |
| PLAT300_ALERT_4_G Atom Site Occupancy of C02C Constrained at | 0.75 Check | |

| | | | | | | | |
|-------------------|--|----------------|-------|-----------|------|------|------|
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02D | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02E | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02F | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02G | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02R | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02P | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02T | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02X | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C02S | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of B02W | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H7 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H8 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H9 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H10 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H11 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H12 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H13 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H22 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H28 | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Ha | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hb | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hc | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hd | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of He | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Ho | Constrained at | 0.75 | Check | | | |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Hp | Constrained at | 0.75 | Check | | | |
| PLAT301_ALERT_3_G | Main Residue Disorder | (Resd 1) | 2% | Note | | | |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder | (Resd 2) | 100% | Note | | | |
| PLAT395_ALERT_2_G | Deviating X-O-Y Angle From 120 for O01V | . | 105.1 | Degree | | | |
| PLAT395_ALERT_2_G | Deviating X-O-Y Angle From 120 for O01X | . | 106.4 | Degree | | | |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn | H1C ..H02D | . | 2.08 Ang. | | | |
| | | x,y,z = | 1_555 | Check | | | |
| PLAT413_ALERT_2_G | Short Inter XH3 .. XHn | H5 ..H12 | . | 2.14 Ang. | | | |
| | | x,y,z = | 1_555 | Check | | | |
| PLAT605_ALERT_4_G | Largest Solvent Accessible VOID in the Structure | | 93 | A**3 | | | |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | 172 | Note | | | |
| Pb01 | Pb02 | Pb03 | A100 | S00C | S00D | 00F | OOG |
| O0H | O0I | O0J | O0K | O0L | O00M | H00M | O0N |
| O0O | O0P | O0Q | O0R | O00S | O00T | O00U | O00V |
| O00W | H00W | O00X | O00Y | O00Z | O010 | O011 | C012 |
| O013 | O014 | O015 | C016 | H016 | C019 | C01B | H01B |
| N01C | C01D | H01D | O01E | C01G | C01I | H01I | C01K |
| H01A | H01C | H01E | C01O | H01O | C01M | H01M | C017 |
| C01A | H01F | C01J | H01J | C01L | C01P | H01G | H01H |
| H01K | C01R | H01R | N01S | N01T | O01V | C01W | H01L |
| H01N | H01P | O01X | C01Y | H01Y | C01U | C022 | H022 |
| C029 | H029 | C025 | C026 | H026 | S01Z | C020 | H02A |
| H02B | H02C | C021 | H02D | H02E | C023 | H023 | C01Q |
| H01Q | C018 | C01F | H01S | C01H | H01T | C01N | C024 |
| H02F | H02G | H02H | C027 | H02I | H02J | H02K | C028 |
| H02L | H02M | C02A | H02N | H02O | H02P | C02B | H02Q |
| H02R | C02C | Ha | C02D | Hb | Hc | C02E | Hd |
| He | C02F | C02G | C02H | H02S | H02T | C02I | H02U |
| H02V | H02W | C02J | H02X | H02Y | C02K | H02Z | Hf |
| Hg | C02L | H02 | Hh | C02M | Hi | C02N | Hj |
| Hk | C02O | H1 | C02Q | Hm | Hn | C02R | C02P |

| | C02T | C02X | C02S | Ho | Hp | C02U | Hq | Hr |
|-------------------|--|-------|-------|-------|-------|------|-----|-----------|
| | C02V | Hs | Ht | B02W | | | | |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -PB02 | 2_665 | 1_555 | 1_555 | | # | 221 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -PB02 | 3_655 | 1_555 | 1_555 | | # | 222 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -PB02 | 4_565 | 1_555 | 1_555 | | # | 223 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 4_565 | 1_555 | 1_555 | | # | 224 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 2_665 | 1_555 | 4_565 | | # | 225 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 3_655 | 1_555 | 3_655 | | # | 226 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 2_665 | 1_555 | 2_665 | | # | 227 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 4_565 | 1_555 | 3_655 | | # | 228 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 2_665 | 1_555 | 3_655 | | # | 229 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 2_665 | 1_555 | 1_555 | | # | 230 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 3_655 | 1_555 | 1_555 | | # | 231 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 4_565 | 1_555 | 4_565 | | # | 232 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 3_655 | 1_555 | 2_665 | | # | 233 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 4_565 | 1_555 | 2_665 | | # | 234 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -AL00 | 3_655 | 1_555 | 4_565 | | # | 235 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -000 | 4_565 | 1_555 | 2_665 | | # | 236 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -000 | 4_565 | 1_555 | 3_655 | | # | 237 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF | ... | | | | | | 0.00 Deg. |
| | 000 -000 -000 | 3_655 | 1_555 | 2_665 | | # | 238 | Check |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Pb02 | (II) | . | . | | | | 2.00 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Pb03 | (II) | . | . | | | | 2.08 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al00 | (III) | . | . | | | | 2.74 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al12 | (III) | . | . | | | | 2.77 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al14 | (III) | . | . | | | | 2.76 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al15 | (III) | . | . | | | | 2.80 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al16 | (III) | . | . | | | | 2.81 Info |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Al17 | (III) | . | . | | | | 2.79 Info |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | | | | | | | 562 Note |
| PLAT868_ALERT_4_G | ALERTS Due to the Use of _smtbx_masks Suppressed | | | | | | | ! Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | | | | | | | 1 Note |
| | 1 1 0, | | | | | | | |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | | | | | | | 539 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 | | | | | | | 49 Note |
| | -3 4 1, 2 2 3, -6 7 3, 15 32 10, -5 7 3, 1 14 6, | | | | | | | |
| | -2 5 2, 0 2 0, 1 3 2, -6 8 0, 1 2 5, 0 8 2, | | | | | | | |
| | 2 4 2, 2 2 0, 0 3 2, -6 9 2, 3 3 4, -3 6 2, | | | | | | | |

```

-2 7 4,   6 9 6,  -1 9 2,  -2 10 2,  -2 5 3,  3 3 0,
-3 13 6,  -1 8 6,  0 4 1,  4 4 2,  -5 11 7,  0 11 4,
 1 6 4,  -5 9 2,  6 9 2,  9 12 6,  -3 8 6,  9 11 1,
 2 7 5,  0 15 6,  -1 3 0,  -6 7 1,  0 9 1,  3 7 5,
-1 7 2,  0 0 2,  0 1 2,  0 2 3,  4 9 6,  1 6 1,
-4 5 8,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.810 Note
Predicted wR2: Based on SigI**2 5.20 or SHELX Weight 18.56
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT984_ALERT_1_G The C-f' = 0.0150 Deviates from the B&C-Value 0.0137 Check
PLAT984_ALERT_1_G The Al-f' = 0.1760 Deviates from the B&C-Value 0.1771 Check
PLAT984_ALERT_1_G The O-f' = 0.0410 Deviates from the B&C-Value 0.0389 Check
PLAT984_ALERT_1_G The Pb-f' = -4.2650 Deviates from the B&C-Value -4.4950 Check
PLAT985_ALERT_1_G The Al-f" = 0.1840 Deviates from the B&C-Value 0.1873 Check
PLAT985_ALERT_1_G The Pb-f" = 7.1980 Deviates from the B&C-Value 6.8412 Check
PLAT985_ALERT_1_G The S-f" = 0.4240 Deviates from the B&C-Value 0.4295 Check

```

```

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

```

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11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
44 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
61 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 SAIOC-1@G9 - ellipsoid plot

