checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ba15_0ma_a

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: ba15_0ma_a

Bond precision: C-C = 0.0075 A Wavelength=1.54178

Cell: a=20.3622(12) b=21.7763(13) c=16.1653(9)
alpha=90 beta=100.835(3) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	7040.1(7)	7040.1(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H30 Br4 N4 O2 Zn, C2 H6 O S	C26 H30 Br4 N4 O2 Zn, C2 H6 O S
Sum formula	C28 H36 Br4 N4 O3 S Zn	C28 H36 Br4 N4 O3 S Zn
Mr	893.66	893.68
Dx,g cm-3	1.686	1.686
Z	8	8
Mu (mm-1)	7.114	7.114
F000	3536.0	3536.0
F000'	3510.56	
h,k,lmax	25,26,19	25,26,19
Nref	13939	13234
Tmin,Tmax	0.483,0.742	0.483,0.742
Tmin'	0.347	

Correction method= # Reported T Limits: Tmin=0.483 Tmax=0.742
AbsCorr = MULTI-SCAN

Data completeness= 0.949 Theta(max)= 72.464

R(reflections)= 0.0570(11999) wR2(reflections)= 0.1511(13234)

S = 1.108 Npar= 762

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

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PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
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Author Response: It may be due to presence of some overlaped reflections that we could not avoid during refinement.

Alert level C

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.140
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.969 Why?
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        O66 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C67 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C68 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C71 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C72 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      S65A      0.158 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      S69A      0.160 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00748 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         65 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.460 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        390 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....         25 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      34.63 Check
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.140 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      11.51 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of S65A       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S65B       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67A       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67B       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67C       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68A       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68B       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68C       Constrained at     0.5769 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67D       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67E       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67F       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68D       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68E       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68F       Constrained at      0.423 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S69A       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S69B       Constrained at     0.3327 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H71A       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71B       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71C       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72A       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72B       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72C       Constrained at     0.6673 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71D       Constrained at     0.3327 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71E       Constrained at     0.3327 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71F       Constrained at     0.3327 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72D       Constrained at     0.3327 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72E       Constrained at     0.3327 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72F       Constrained at     0.3327 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        25% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        25% Note
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.14910 Dev...       0.19 Ang.
              C68      -H68D           1_555   1_555 ........     #  155 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.07810 Dev...       0.12 Ang.
              C68      -H68E           1_555   1_555 ........     #  156 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.15010 Dev...       0.19 Ang.
              C68      -H68F           1_555   1_555 ........     #  157 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.98980 Dev...       0.03 Ang.
              C67      -H67D           1_555   1_555 ........     #  163 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.98930 Dev...       0.03 Ang.
              C67      -H67E           1_555   1_555 ........     #  164 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.98900 Dev...       0.03 Ang.
              C67      -H67F           1_555   1_555 ........     #  165 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.00290 Dev...       0.04 Ang.
              C67      -H67A           1_555   1_555 ........     #  166 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.11700 Dev...       0.16 Ang.
              C67      -H67B           1_555   1_555 ........     #  167 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.04820 Dev...       0.09 Ang.
              C67      -H67C           1_555   1_555 ........     #  168 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97910 Dev...       0.02 Ang.
              C71      -H71D           1_555   1_555 ........     #  174 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97940 Dev...       0.02 Ang.
              C71      -H71E           1_555   1_555 ........     #  175 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     0.97900 Dev...       0.02 Ang.
              C71      -H71F           1_555   1_555 ........     #  176 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.22420 Dev...       0.26 Ang.
              C72      -H72D           1_555   1_555 ........     #  182 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.01540 Dev...       0.06 Ang.
              C72      -H72E           1_555   1_555 ........     #  183 Check
PLAT721_ALERT_1_G Bond    Calc     0.96000, Rep     1.02790 Dev...       0.07 Ang.
              C72      -H72F           1_555   1_555 ........     #  184 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      154.50 Dev...      45.50 Degree
              S65B    -C68     -H68D       1_555  1_555  1_555     #  299 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep       86.60 Dev...      22.40 Degree
              S65B    -C68     -H68E       1_555  1_555  1_555     #  300 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      113.00 Dev...       3.00 Degree
              H68D    -C68     -H68E       1_555  1_555  1_555     #  301 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep       86.70 Dev...      22.30 Degree
              S65B    -C68     -H68F       1_555  1_555  1_555     #  302 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep       97.70 Dev...      12.30 Degree
              H68D    -C68     -H68F       1_555  1_555  1_555     #  303 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      116.90 Dev...       7.90 Degree
              H68E    -C68     -H68F       1_555  1_555  1_555     #  304 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      112.30 Dev...       3.30 Degree
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              S65B    -C67     -H67D       1_555  1_555  1_555     #  311 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      112.20 Dev...       3.20 Degree
              S65B    -C67     -H67E       1_555  1_555  1_555     #  312 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      106.60 Dev...       3.40 Degree
              H67D    -C67     -H67E       1_555  1_555  1_555     #  313 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      112.00 Dev...       3.00 Degree
              S65B    -C67     -H67F       1_555  1_555  1_555     #  314 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      106.70 Dev...       2.30 Degree
              H67D    -C67     -H67F       1_555  1_555  1_555     #  315 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      106.70 Dev...       3.30 Degree
              H67E    -C67     -H67F       1_555  1_555  1_555     #  316 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      157.80 Dev...      48.80 Degree
              S65A    -C67     -H67A       1_555  1_555  1_555     #  317 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep       89.00 Dev...      20.00 Degree
              S65A    -C67     -H67B       1_555  1_555  1_555     #  318 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      113.20 Dev...       3.20 Degree
              H67A    -C67     -H67B       1_555  1_555  1_555     #  319 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep       72.90 Dev...      36.10 Degree
              S65A    -C67     -H67C       1_555  1_555  1_555     #  320 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep       96.40 Dev...      13.60 Degree
              H67A    -C67     -H67C       1_555  1_555  1_555     #  321 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      113.30 Dev...       4.30 Degree
              H67B    -C67     -H67C       1_555  1_555  1_555     #  322 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      106.30 Dev...       2.70 Degree
              S69A    -C71     -H71A       1_555  1_555  1_555     #  323 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      112.60 Dev...       3.60 Degree
              S69A    -C71     -H71B       1_555  1_555  1_555     #  324 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      110.40 Dev...       1.40 Degree
              S69A    -C71     -H71C       1_555  1_555  1_555     #  326 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      108.50 Dev...       1.50 Degree
              H71B    -C71     -H71C       1_555  1_555  1_555     #  328 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      111.40 Dev...       2.40 Degree
              S69B    -C71     -H71D       1_555  1_555  1_555     #  329 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      111.50 Dev...       2.50 Degree
              S69B    -C71     -H71E       1_555  1_555  1_555     #  330 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      107.50 Dev...       2.50 Degree
              H71D    -C71     -H71E       1_555  1_555  1_555     #  331 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      111.30 Dev...       2.30 Degree
              S69B    -C71     -H71F       1_555  1_555  1_555     #  332 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      107.50 Dev...       2.50 Degree
              H71D    -C71     -H71F       1_555  1_555  1_555     #  333 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      107.40 Dev...       2.60 Degree
              H71E    -C71     -H71F       1_555  1_555  1_555     #  334 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      145.60 Dev...      35.60 Degree
              S69B    -C72     -H72D       1_555  1_555  1_555     #  341 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep       82.00 Dev...      27.00 Degree
              S69B    -C72     -H72E       1_555  1_555  1_555     #  342 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      104.10 Dev...       4.90 Degree
              H72D    -C72     -H72E       1_555  1_555  1_555     #  343 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      101.70 Dev...       8.30 Degree
              S69B    -C72     -H72F       1_555  1_555  1_555     #  344 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      107.00 Dev...       2.00 Degree
              H72D    -C72     -H72F       1_555  1_555  1_555     #  345 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      111.80 Dev...       2.80 Degree
              H72E    -C72     -H72F       1_555  1_555  1_555     #  346 Check
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at N17         (Centro SPGR)          R Verify
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PLAT793_ALERT_4_G Model has Chirality at N33         (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N49         (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C22         (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C38         (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C54         (Centro SPGR)          R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       1.96 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        316 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  96 ALERT level G = General information/check it is not something unexpected

  51 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
  44 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock ba15_0ma_a - ellipsoid plot