checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: a_a_sq

Bond precision: C-C = 0.0105 A Wavelength=0.71073

Cell: a=25.514(10) b=33.507(10) c=18.134(7)
alpha=90 beta=114.809(14) gamma=90
Temperature: 273 K

	Calculated	Reported
Volume	14072(9)	14072(9)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C40 H44 N24 O12), Cl7 Zn2, 2(C7 H7 N2), 2(Cl4 Zn), 4(H2 O) [+	Cl4 Zn, Cl3.5 Zn, C40 H44 N24 O12, C7 H7 N2, 2(H2 O)
Sum formula	C94 H110 Cl15 N52 O28 Zn4 [+ solvent]	C47 H55 Cl7.50 N26 O14 Zn2
Mr	3209.65	1604.78
Dx,g cm-3	1.515	1.515
Z	4	8
Mu (mm-1)	1.043	1.043
F000	6548.0	6548.0
F000'	6563.52	
h,k,lmax	30,39,21	30,39,21
Nref	12391	12365
Tmin,Tmax	0.901,0.911	0.559,0.746
Tmin'	0.901	

Correction method= # Reported T Limits: Tmin=0.559 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0724(6681)

wR2(reflections)= 0.2303(12365)

S = 1.004 Npar= 875

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

PLAT334_ALERT_2_B Small Aver. Benzene C-C Dist C42 -C44 1.34 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H14D ..H26A . 1.91 Ang.
x,y,z = 1_555 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D H14E ..H26A . 2.07 Ang.
x,y,z = 1_555 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor O13 --H13B . Please Check

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Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for O4 --C32 . 5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N12 --C20 . 5.7 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) N26 --C46 . 7.3 s.u.
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C43 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C44 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C45 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C47 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Zn1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C41 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C42 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Zn2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O13 0.181 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01053 Ang.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 7 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 273 Check
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) N25 --C41 . 6.7 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C41 --C42 . 5.7 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl4 ..C6 . 3.24 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
Cl4 Zn
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 2.04 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.8 Low

PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree

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

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2 ALERT type 3 Indicator that the structure quality may be low
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4 ALERT type 5 Informative message, check

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Publication of your CIF in IUCr journals

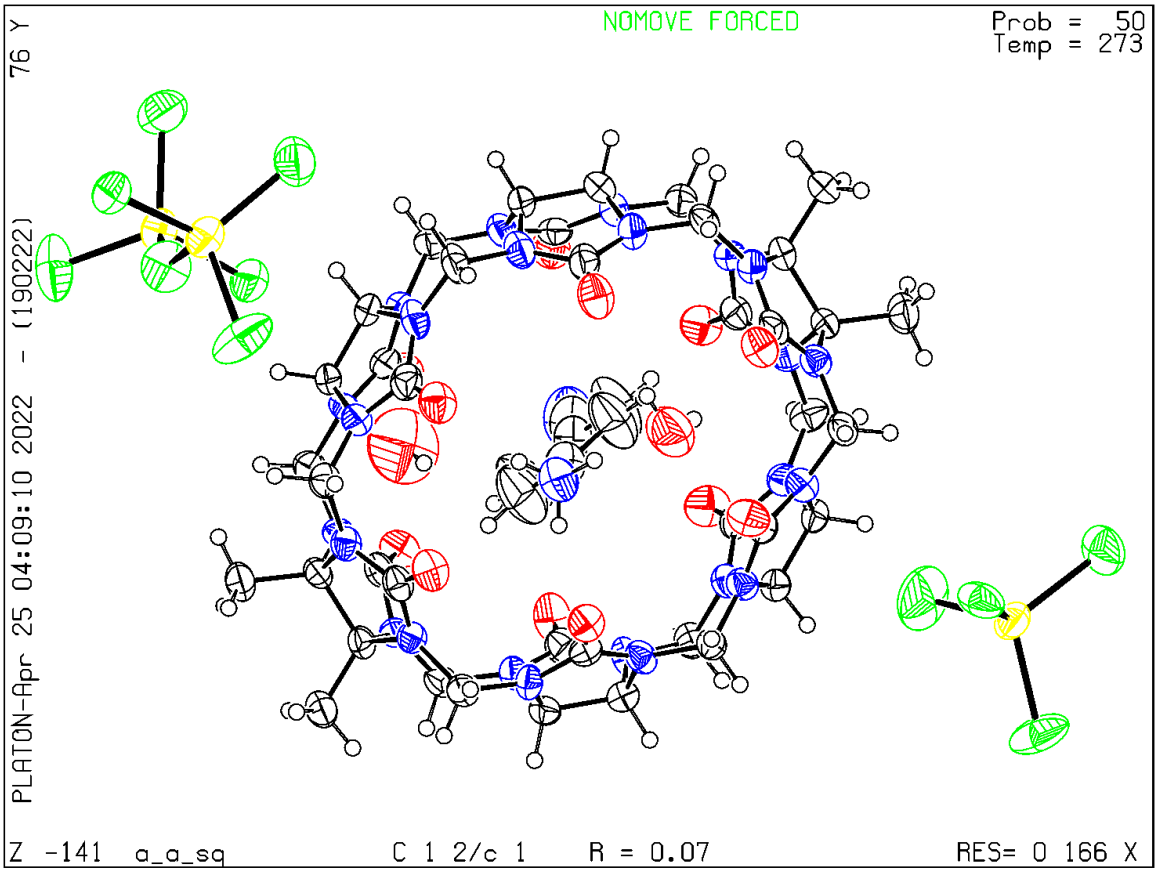
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/02/2022; check.def file version of 19/02/2022

Datablock a_a_sq - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: a_a_sq

```
Bond precision:  C-C = 0.0171 A          Wavelength=0.71073

Cell:          a=16.196(4)       b=21.572(6)      c=24.111(7)
               alpha=92.944(8)   beta=98.870(8)   gamma=109.924(7)
Temperature:   273 K
```

	Calculated	Reported
Volume	7776(4)	7776(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H44 N24 O12, 2(C13 H16 N2), 2(Cl4 Zn) [+ solvent]	2(Cl4 Zn), C40 H44 N24 O12, 2(C13 H16 N2)
Sum formula	C66 H76 Cl8 N28 O12 Zn2 [+ solvent]	C66 H76 Cl8 N28 O12 Zn2
Mr	1867.93	1867.88
Dx,g cm-3	1.197	1.197
Z	3	3
Mu (mm-1)	0.729	0.729
F000	2880.0	2880.0
F000’	2886.12	
h,k,lmax	19,25,28	19,25,28
Nref	27401	27326
Tmin,Tmax	0.896,0.916	0.603,0.746
Tmin’	0.896	

```
Correction method= # Reported T Limits: Tmin=0.603 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.000

R(reflections)= 0.1254( 11486)    wR2(reflections)= 0.3809( 27326)

S = 1.073                 Npar= 1586
```

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.38 Report
PLAT230_ALERT_2_B Hirshfeld Test Diff for N23 --C1 . 8.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C14 --C16 . 12.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C15 --C17 . 17.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N0AA --C71 . 13.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for N41 --C61 . 9.6 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C61 --C66 . 8.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C68 --C69 . 7.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C68 --C73 . 9.7 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference C65 --C66 . 0.29 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C68 Check
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01711 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H11A ..H14B . 1.70 Ang.
x,y,z = 1_555 Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.164
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.164 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT082_ALERT_2_C High R1 Value ..... 0.13 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N4 --C10 . 6.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N10 --C20 . 5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N13 --C21 . 5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N25 --C43 . 6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C48 --C49 . 5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C51 --C53 . 6.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C64 --C67 . 5.8 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4 --C13 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5 --C21 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O7 --C4 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O11 --C18 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C3 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3 --C5 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5 --C9 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6 --C9 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6 --C10 . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N7 --C11 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C12 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C16 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C18 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9 --C13 . 0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9 --C17 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9 --C19 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N10 --C17 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N11 --C19 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N11 --C22 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N14 --C26 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N15 --C27 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N17 --C27 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N19 --C31 . 0.17 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference N21      --C39      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N22      --C02H     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N23      --C2       .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C02H     --C36      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22      --C23      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O15      --C50      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O16      --C52      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N27      --C45      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N36      --C60      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43      --C44      .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C64      --C65      .       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C90      --C91      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C91      --C92      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C97      --C98      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C77      --C78      .       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C12 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        C63 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C67 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C69 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C73 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C93 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C02H Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C17 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C53 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C64 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C71 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C87 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C90 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        Cl9 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       Cl12 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Zn2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      N0AA      0.184 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Zn4      0.176 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Zn2      0.153 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C87      -C92            1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C74      -C79            1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C81      -C86            1.37 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C67      - C68      .       1.37 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N0AA     --H0AA     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N0AA     --H0AB     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N0AA     --H0AC     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N37      --H37A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N37      --H37B     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N37      --H37C     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N38      --H38B     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N40      --H40E     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N41      --H41C     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N41      --H41D     .     Please Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         8 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        20 Report
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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............        12 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.20 Report
PLAT073_ALERT_1_G H-atoms ref, but _hydrogen_treatment Reported as     constr Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          7 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          5 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       273 Check
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Zn4      --Cl9      .       35.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Zn4      --Cl12     .       27.5 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Zn4      --Cl13     .       43.7 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Zn3      --Cl9      .       13.8 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Zn3      --Cl12     .       14.2 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       40% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........         ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         5 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      0.00 Deg.
             H0AA -N0AA -H0AA    1_555   1_555   1_555 ......     #  599 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      0.00 Deg.
             H0AB -N0AA -H0AB    1_555   1_555   1_555 ......     #  607 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      0.00 Deg.
             H0AC -N0AA -H0AC    1_555   1_555   1_555 ......     #  615 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3 Note
             C13 H16 N2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         7 Note
             Cl4 Zn
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         8 Note
             Cl4 Zn
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       2.04 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       129 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        44 Note
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  7 ALERT type 3 Indicator that the structure quality may be low
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  3 ALERT type 5 Informative message, check

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Publication of your CIF in IUCr journals

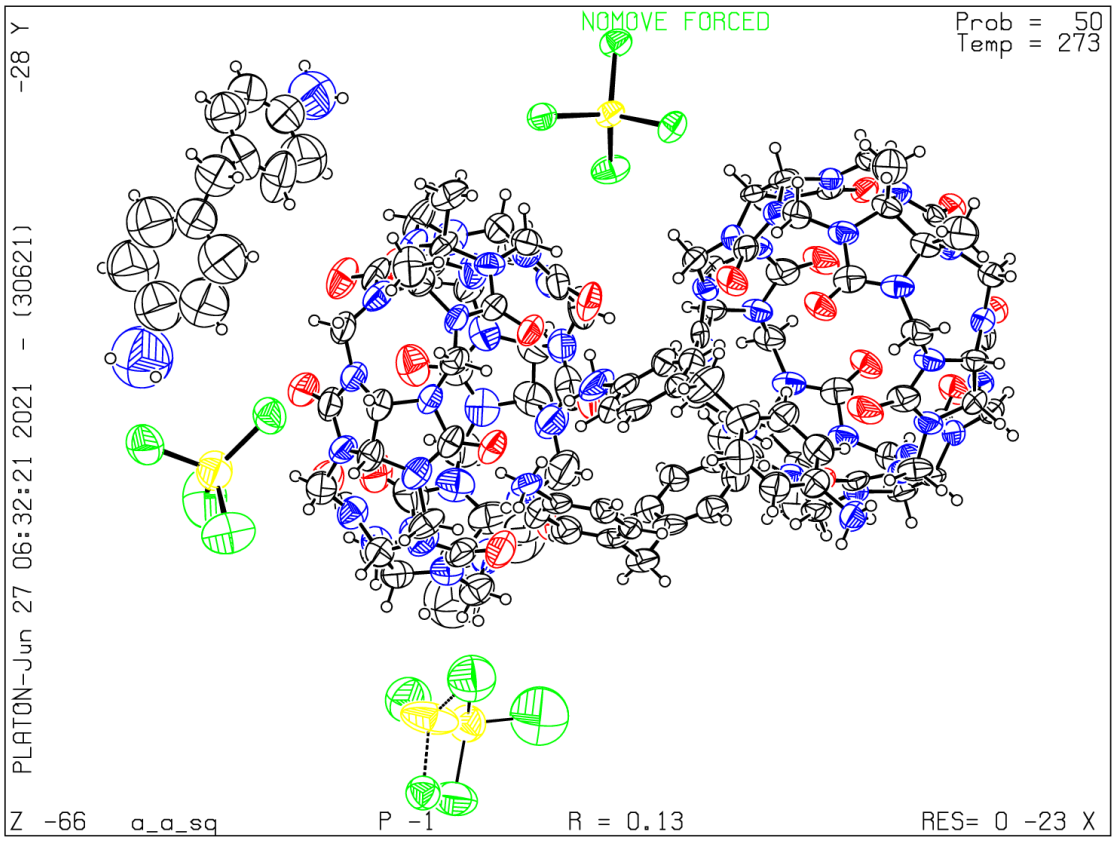
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/06/2021; check.def file version of 02/06/2021

Datablock a_a_sq - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: a_a_sq

Bond precision: C-C = 0.0103 A Wavelength=0.71073

Cell: a=12.982(5) b=25.563(10) c=28.478(12)
alpha=112.834(12) beta=90.524(12) gamma=93.767(13)
Temperature: 273 K

	Calculated	Reported
Volume	8685(6)	8685(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C40 H44 N24 O12), 3(C13 H14 N), 3(Cl4 Zn), 2(H2 O) [+ solvent	3(Cl4 Zn), 2(C40 H44 N24 O12), 3(C13 H14 N), 2(H2 O)
Sum formula	C119 H134 Cl12 N51 O26 Zn3 [+ solvent]	C119 H134 Cl12 N51 O26 Zn3
Mr	3316.35	3316.27
Dx,g cm-3	1.268	1.268
Z	2	2
Mu (mm-1)	0.668	0.668
F000	3414.0	3414.0
F000'	3420.39	
h,k,lmax	15,30,33	15,30,33
Nref	30601	30420
Tmin,Tmax	0.935,0.938	0.402,0.746
Tmin'	0.935	

Correction method= # Reported T Limits: Tmin=0.402 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.000

R(reflections)= 0.0824(15420)

wR2(reflections)= 0.2487(30420)

S = 1.020 Npar= 1890

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 C

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O7       --C39      .        5.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N15      --C20      .        5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O20      --C53      .        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N51      --C107     .        5.7 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C87 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C95 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C99 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C100 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C97 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C110 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Zn3 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Zn1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Zn2 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N51      0.124 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Zn2      0.128 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C88      -C93            1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01031 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H43      ..H0AB     .       2.04 Ang.
                                            -1+x,-1+y,z  =      1_445 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N51      --H        .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N49      --H02E     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N50      --H02I     .     Please Check
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         12 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         13 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.12 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       273 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       126 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             Cl4 Zn
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       2.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       2.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn3       (II)      .       2.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       105 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

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PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        2.8 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
```

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 19/02/2022; check.def file version of 19/02/2022

Datablock a_a_sq - ellipsoid plot