# checkCIF/PLATON report

Supplementary Material (ESI) for Chemical Communications


**No syntax errors found.** **CIF dictionary** **Interpreting this report**

## Datablock: 2_ZnL.MeOH

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**Bond precision: C-C = 0.0048 A Wavelength=0.71073**

**Cell: a=17.428(4) b=13.517(3) c=17.588(4)**
**alpha=90 beta=100.24(3) gamma=90**
**Temperature: 293 K**

| | Calculated | Reported |
|---|---|---|
| Volume | 4077.3(16) | 4077.5(14) |
| Space group | P 21 | P2(1) |
| Hall group | P 2yb | ? |
| Moiety formula | C42 H46 N4 O2 Zn, C H4 O | ? |
| Sum formula | C43 H50 N4 O3 Zn | C86 H100 N8 O6 Zn2 |
| Mr | 736.26 | 1472.48 |
| Dx,g cm-3 | 1.199 | 1.199 |
| Z | 4 | 2 |
| Mu (mm-1) | 0.644 | 0.644 |
| F000 | 1560.0 | 1560.0 |
| F000' | 1561.64 | |
| h,k,lmax | 20,16,20 | 20,16,20 |
| Nref | 7512[ 14360] | 12720 |
| Tmin,Tmax | 0.911,0.938 | 0.900,0.920 |
| Tmin' | 0.908 | |

**Correction method= MULTI-SCAN**

**Data completeness= 1.69/0.89 Theta(max)= 25.000**

**R(reflections)= 0.0720( 7056) wR2(reflections)= 0.2292( 12720)**

**S = 1.065 Npar= 796**

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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.

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### Alert level A

PLAT213_ALERT_2_A Atom C16 has ADP max/min Ratio ..... 5.20 prola
PLAT213_ALERT_2_A Atom C84 has ADP max/min Ratio ..... 5.50 prola
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.70 Ratio
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 7.91 Ratio
PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for C83
PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for C84

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PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C14
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C32
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C80
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for        C81
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## Alert level B

```
PLAT111_ALERT_2_B ADDSYM Detects (Pseudo) Centre of Symmetry .....         90 PerFi
PLAT213_ALERT_2_B Atom C15            has ADP max/min Ratio .....       4.60 prola
PLAT213_ALERT_2_B Atom C57            has ADP max/min Ratio .....       4.70 prola
PLAT220_ALERT_2_B Large Non-Solvent    N     Ueq(max)/Ueq(min) ...       4.51 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O2     --  C27     ..      22.80 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N2     --  C19     ..       9.91 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N4     --  C40     ..      10.28 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C2     --  C3      ..       8.45 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C9     --  C10     ..       7.05 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C10    --  C18     ..       7.84 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C11    --  C12     ..      20.03 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C14    --  C16     ..      12.98 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C25    --  C26     ..       7.35 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C28    --  C36     ..      10.43 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C29    --  C30     ..      11.42 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C36    --  C37     ..      12.73 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O3     --  C51     ..      16.58 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O4     --  C69     ..      13.39 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N6     --  C60     ..       8.64 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    N8     --  C82     ..      12.08 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C46    --  C47     ..      10.09 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C51    --  C52     ..       7.73 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C54    --  C55     ..       7.49 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C61    --  C66     ..      19.88 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C63    --  C64     ..       8.87 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C68    --  C69     ..      15.01 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C69    --  C70     ..       7.51 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C78    --  C79     ..      10.69 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C80    --  C81     ..      10.05 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C80    --  C84     ..      13.01 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C81    --  C82     ..       7.18 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C83    --  C84     ..       8.97 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Zn1    --  N2      ..      13.40 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Zn2    --  O3      ..      10.13 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Zn2    --  O4      ..      10.98 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X)  Zn2    --  N5_c    ..      13.64 su
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for         N8
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C56
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C74
PLAT412_ALERT_2_B Short Intra XH3 .. XHn     H58C   ..  H59B    ..       1.79 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H34C   ..  H85A    ..       2.01 Ang.
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## Alert level C

```
CELLV02_ALERT_1_C  The supplied cell volume s.u. differs from that
           calculated from the cell parameter s.u.'s by > 2
           Calculated cell volume su =      16.44
           Cell volume su given      =      14.00
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          4
PLAT213_ALERT_2_C Atom C33            has ADP max/min Ratio .....       3.20 prola
PLAT213_ALERT_2_C Atom N8             has ADP max/min Ratio .....       3.10 prola
PLAT213_ALERT_2_C Atom C83            has ADP max/min Ratio .....       3.50 prola
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uso(min) ...       6.64 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uso(min) ...       6.75 Ratio
```

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1    --  O3      ..       5.68 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1    --  C1      ..       6.73 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N3    --  C25     ..       6.87 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C3    --  C4      ..       5.84 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C6    --  C7      ..       6.48 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C26   --  C31     ..       5.28 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C32   --  C34     ..       6.72 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C38   --  C42     ..       6.43 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N7    --  C67     ..       5.74 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C43   --  C44     ..       5.28 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C44   --  C45     ..       5.59 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45   --  C46     ..       5.66 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C50   --  C55     ..       6.28 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C62   --  C63     ..       6.84 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C67   --  C68     ..       5.05 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C71   --  C72     ..       6.66 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn1   --  O2      ..       9.44 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn1   --  N3      ..       7.53 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn2   --  N7      ..       5.07 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C5
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C42
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C47
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C3
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N5
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C54
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.13
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C14   -   C15   ...      1.43 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H5A   ..  H85C   ..      2.14 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .     34.00 A**3
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ        ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............      2.00 Ratio
PLAT152_ALERT_1_C The Supplied and Calc. Volume s.u. Differ by ...         2 Units
PLAT234_ALERT_4_C Large Hirshfeld Difference N8    --  C83     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C56   --  C57     ..      0.16 Ang.
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### Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max          25.00
          From the CIF: _reflns_number_total             12720
          Count of symmetry unique reflns         7512
          Completeness (_total/calc)           169.33%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      5208
          Fraction of Friedel pairs measured     0.693
          Are heavy atom types Z>Si present        yes
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.12
PLAT343_ALERT_2_G Check sp3     Angle Range in Main Residue for ..       C56
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        20
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT791_ALERT_4_G Note: The Model has Chirality at C19    (Verify)         R
PLAT791_ALERT_4_G Note: The Model has Chirality at C24    (Verify)         R
PLAT791_ALERT_4_G Note: The Model has Chirality at C61    (Verify)         R
PLAT791_ALERT_4_G Note: The Model has Chirality at C66    (Verify)         R
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Zn1     .......      2.09
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Zn2     .......      2.15
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10 **ALERT level A** = In general: serious problem
41 **ALERT level B** = Potentially serious problem
42 **ALERT level C** = Check and explain
12 **ALERT level G** = General alerts; check

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
86 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
2 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*, 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.

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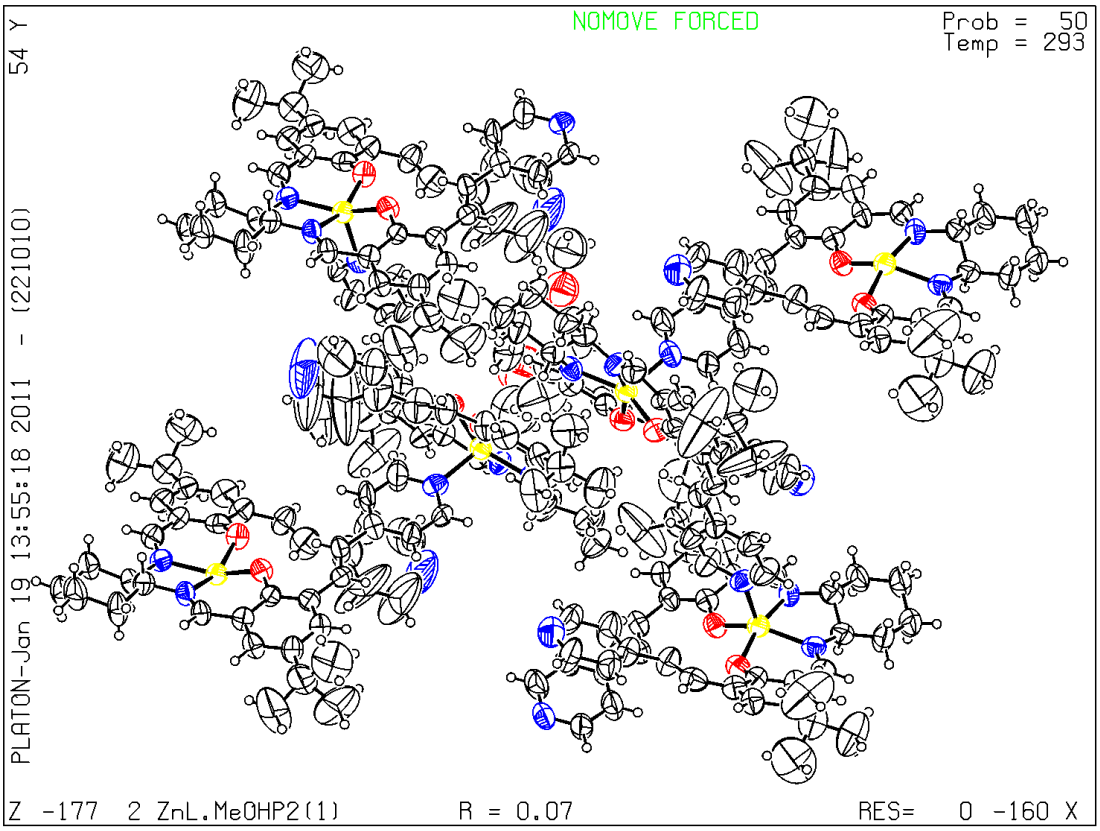
PLATON version of 22/10/2010; check.def file version of 11/10/2010

**Datablock 2_ZnL.MeOH - ellipsoid plot**



# checkCIF/PLATON report

Supplementary Material (ESI) for Chemical Communications


**No syntax errors found.** **CIF dictionary** **Interpreting this report**

## Datablock: 1_ZnL

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**Bond precision: C-C = 0.0155 A Wavelength=0.71073**

**Cell: a=12.616(3) b=25.145(5) c=12.892(3)**
**alpha=90 beta=108.88(3) gamma=90**
**Temperature: 293 K**

| | Calculated | Reported |
|---|---|---|
| Volume | 3869.7(17) | 3869.6(13) |
| Space group | P 21 | P2(1) |
| Hall group | P 2yb | ? |
| Moiety formula | C84 H92 N8 O4 Zn2 | ? |
| Sum formula | C84 H92 N8 O4 Zn2 | C84 H92 N8 O4 Zn2 |
| Mr | 1408.44 | 1408.40 |
| Dx,g cm-3 | 1.209 | 1.209 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.673 | 0.673 |
| F000 | 1488.0 | 1488.0 |
| F000' | 1489.59 | |
| h,k,lmax | 15,29,15 | 14,29,15 |
| Nref | 6983[ 13625] | 11968 |
| Tmin,Tmax | 0.922,0.948 | 0.900,0.920 |
| Tmin' | 0.922 | |

**Correction method= MULTI-SCAN**

**Data completeness= 1.71/0.88 Theta(max)= 25.000**

**R(reflections)= 0.0744( 6620) wR2(reflections)= 0.1501( 11968)**

**S = 1.019 Npar= 787**

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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.

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**Alert level A**

PLAT213_ALERT_2_A Atom C75 has ADP max/min Ratio ..... 5.90 prola
PLAT213_ALERT_2_A Atom C76 has ADP max/min Ratio ..... 5.20 prola
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 7.52 Ratio
PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C14
PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C56
PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C74

## Alert level B

```
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low .....       0.96
PLAT213_ALERT_2_B Atom C77            has ADP max/min Ratio .....      4.60 prola
PLAT222_ALERT_3_B Large Non-Solvent    H    Uiso(max)/Uso(min) ...      8.56 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C72    --  C78     ..      9.45 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C78    --  C79     ..      8.50 su
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C41
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C84
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        C32
PLAT115_ALERT_5_B ADDSYM Detects Noncrystallographic Inversion ...        87 PerFi
PLAT234_ALERT_4_B Large Hirshfeld Difference N4     --  C40     ..      0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C74    --  C76     ..      0.28 Ang.
```

## Alert level C

```
CELLV02_ALERT_1_C  The supplied cell volume s.u. differs from that
           calculated from the cell parameter s.u.'s by > 2
           Calculated cell volume su =      16.52
           Cell volume su given      =      13.00
PLAT213_ALERT_2_C Atom C16            has ADP max/min Ratio .....      3.80 prola
PLAT213_ALERT_2_C Atom C17            has ADP max/min Ratio .....      3.60 prola
PLAT213_ALERT_2_C Atom C74            has ADP max/min Ratio .....      3.80 prola
PLAT213_ALERT_2_C Atom C78            has ADP max/min Ratio .....      3.80 prola
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C36    --  C37     ..      5.89 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C71
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N5
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C39
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C54
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C70
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C72
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..        15
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C14    -   C15    ...      1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C56    -   C59    ...      1.41 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C72    -   C78    ...      1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C79    -   C80    ...      1.54 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H17A   ..  H62B    ..      2.13 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H46A   ..  H75A    ..      2.10 Ang.
PLAT152_ALERT_1_C The Supplied and Calc. Volume s.u. Differ by ...         4 Units
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  C19     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4     --  C41     ..      0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1     --  C2      ..      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7     --  C8      ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9     --  C10     ..      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27    --  C28     ..      0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28    --  C29     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29    --  C30     ..      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30    --  C31     ..      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30    --  C32     ..      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32    --  C35     ..      0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C38    --  C39     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C50    --  C51     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C52    --  C60     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53    --  C54     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C54    --  C56     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C79    --  C80     ..      0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C81    --  C82     ..      0.19 Ang.
```

## Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
```

```
 _publ_section_exptl_refinement section of the submitted CIF:
From the CIF: _diffrn_reflns_theta_max                25.00
From the CIF: _reflns_number_total                    11968
Count of symmetry unique reflns                       6983
Completeness (_total/calc)                            171.39%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured                    4985
Fraction of Friedel pairs measured                    0.714
Are heavy atom types Z>Si present                     yes
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          8
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT791_ALERT_4_G Note: The Model has Chirality at C19    (Verify)          R
PLAT791_ALERT_4_G Note: The Model has Chirality at C24    (Verify)          R
PLAT791_ALERT_4_G Note: The Model has Chirality at C61    (Verify)          R
PLAT791_ALERT_4_G Note: The Model has Chirality at C66    (Verify)          R
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Zn1     .......       2.18
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Zn2     .......       2.17
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```
   6 ALERT level A = In general: serious problem
  11 ALERT level B = Potentially serious problem
  38 ALERT level C = Check and explain
  10 ALERT level G = General alerts; check

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

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**PLATON version of 22/10/2010; check.def file version of 11/10/2010**

**Datablock 1_ZnL - ellipsoid plot**