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: MT119B

```
Bond precision:   C-C = 0.0056 A            Wavelength=0.71073

Cell:             a=29.161(3)     b=30.102(3)          c=31.045(3)
                  alpha=90        beta=102.323(2)      gamma=90
Temperature:      100 K

                  Calculated              Reported
Volume            26624(5)                26624(5)
Space group       C 2/c                   C 2/c
Hall group        -C 2yc                  -C 2yc
Moiety formula    C144 H204 B6 I6 N36 S18  C144 H204 B6 I6 N36 S18
                  Zn6 [+ solvent]         Zn6
Sum formula       C144 H204 B6 I6 N36 S18  C144 H204 B6 I6 N36 S18
                  Zn6 [+ solvent]         Zn6
Mr                4235.13                 4234.98
Dx,g cm-3         1.057                   1.057
Z                 4                       4
Mu (mm-1)         1.407                   1.407
F000              8544.0                  8544.0
F000'             8550.01
h,k,lmax          35,37,38                35,37,38
Nref              26176                   26154
Tmin,Tmax         0.635,0.713             0.735,1.000
Tmin'             0.622

Correction method= # Reported T Limits: Tmin=0.735 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 26.000

R(reflections)= 0.0399( 19711)    wR2(reflections)= 0.1151( 26154)

S = 1.134                  Npar= 1018
```

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

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range      3.8 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range      4.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C90      --C99     .       5.5 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C65 Check
PLAT245_ALERT_2_C U(iso) H3         Smaller than U(eq) B3      by    0.018 Ang**2
PLAT245_ALERT_2_C U(iso) H65        Smaller than U(eq) C65     by    0.011 Ang**2
```

⚪ Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite     22 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records      8 Report
```

Author Response: Two tert. butyl groups (bonded to C16, C36) were disordered over two orientations and refined with site occupation factors of 0.815(5) and 0.839(4), resp., for the more prominent occupied orientations. The same anisotropic displacement parameters were used for equivalent C atoms of these disordered tert. butyl groups (2*4 EADP instructions of SHELXL) and the C-C distances were restrained to 1.53A (DFIX of SHELXL), The other non-hydrogen atoms of the complex were refined with anisotropic displacement parameters without any constraints.

```
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records      1 Report
```

Author Response: see above.

```
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records      1 Report
```

Author Response: The H atoms bonded to the B atoms could be clearly identified in a difference Fourier map and were refined with a common isotropic displacement parameter. The B-H distances were restrained to have the same lengths (SADI instruction of SHELXL) but these H atoms were refined without any further positional constraints.

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I1       --Zn1    .       6.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ............(Resd  1 )       7% Note
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure   ! Info
```

Author Response: Besides the described hexameric complex there are large regions containing disordered n-hexane molecules. Since it was not possible to describe the refined peaks of residual electron density as partially occupied individual solvent molecules, the diffuse electron density in these regions was calculated by the SQUEEZE routine of the PLATON program (A. L. Spek, 2015). The solvent contribution to the calculated structure factors for each reflection hkl is included in the FAB file. The SQUEEZE routine computed a very large void volume of 9982 A**3 (37.5% of the unit cell) with an electron count of approx. 3586 per unit cell (consistent with 72 n-hexane molecules with 50 electrons each). Further details are given in _refine_special_details.

```
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1      (II)     .      2.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2      (II)     .      2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn3      (II)     .      2.06 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     15 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed       ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      11 Note
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: MR38

```
Bond precision:   C-C = 0.0016 A          Wavelength=0.71073

Cell:            a=10.2147(3)    b=8.6489(2)           c=27.2498(8)
                 alpha=90        beta=96.6196(13)      gamma=90
Temperature:     100 K
```

```
                  Calculated                 Reported
Volume            2391.36(11)                2391.36(11)
Space group       P 21/c                     P 21/c
Hall group        -P 2ybc                    -P 2ybc
Moiety formula    C18 H28 Br2 N4 S2 Zn       C18 H28 Br2 N4 S2 Zn
Sum formula       C18 H28 Br2 N4 S2 Zn       C18 H28 Br2 N4 S2 Zn
Mr                589.75                     589.75
Dx,g cm-3         1.638                      1.638
Z                 4                          4
Mu (mm-1)         4.554                      4.554
F000              1184.0                     1184.0
F000'             1184.18
h,k,lmax          16,13,43                   16,13,43
Nref              10522                      10517
Tmin,Tmax         0.278,0.505                0.736,1.000
Tmin'             0.234

Correction method= # Reported T Limits: Tmin=0.736 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 35.000

R(reflections)= 0.0224( 9146)     wR2(reflections)= 0.0500( 10517)

S = 1.046                  Npar= 268
```

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 G**

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      4 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records      1 Report
```

**Author Response: The positions of the H atoms H12 and H22 were taken
from a difference Fourier map, the N-H distances were fixed to 0.88A, and
these H atoms were refined without any constraints to the bond angles
(DFIX of SHELXL).**

```
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C21 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1      (II)      .    1.96 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............      2 Note
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: MR55B

Bond precision: C-C = 0.0143 A   Wavelength=0.71073

Cell: a=16.6456(19)   b=16.9851(19)   c=34.357(4)
                 alpha=90   beta=90   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	9713.7(19)	9713.6(19)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C36 H54 B Br N8 S4 Zn [+ solvent]	C36 H54 B Br N8 S4 Zn
Sum formula	C36 H54 B Br N8 S4 Zn [+ solvent]	C36 H54 B Br N8 S4 Zn
Mr	883.21	883.20
Dx,g cm-3	1.208	1.208
Z	8	8
Mu (mm-1)	1.532	1.532
F000	3680.0	3680.0
F000'	3684.68	
h,k,lmax	19,20,40	19,20,40
Nref	17106[9331]	16976
Tmin,Tmax	0.755,0.807	0.790,1.000
Tmin'	0.740	

Correction method= # Reported T Limits: Tmin=0.790 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.82/0.99   Theta(max)= 25.000

R(reflections)= 0.0526(11043)   wR2(reflections)= 0.1315(16976)

S = 1.014   Npar= 961

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**
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   3.9 Ratio

```
PLAT220_ALERT_2_C Non-Solvent  Resd 2  C   Ueq(max)/Ueq(min) Range       3.3 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 2  H   Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C10      --C18     .     0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30      --C36     .     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C34      --C35     .     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C35      --C36     .     0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43      --C44     .     0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C45      --C46     .     0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N72      --C73     .     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C50      --C59     .     0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C80      --C88     .     0.16 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C40 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C50 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C60 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C70 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C80 Check
PLAT245_ALERT_2_C U(iso) H1       Smaller than U(eq) B1      by    0.030 Ang**2
PLAT245_ALERT_2_C U(iso) H2       Smaller than U(eq) B2      by    0.031 Ang**2
PLAT245_ALERT_2_C U(iso) H571     Smaller than U(eq) C57     by    0.011 Ang**2
PLAT245_ALERT_2_C U(iso) H572     Smaller than U(eq) C57     by    0.011 Ang**2
PLAT245_ALERT_2_C U(iso) H573     Smaller than U(eq) C57     by    0.011 Ang**2
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.01428 Ang.
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⬤ **Alert level G**
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite     4 Note
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .  0.078 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records      1 Report
```

Author Response: The positions of the H atoms of the NH groups were taken from a difference Fourier map, the N-H distances were fixed to 0.88A, and these H atoms were refined with a common isotropic displacement parameter without any constraints to the bond angles (DFIX of SHELXL).

```
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....    C71 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure     ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1     (II)    .   1.95 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2     (II)    .   1.94 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     2 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed     ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...     7 Note
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 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
  14 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 13/12/2018; check.def file version of 11/12/2018

NOMOVE FORCED

Prob = 50
Temp = 100

63 Y

PLATON-Dec 19 09:42:01 2018 - (70316)

Z -59   MR55B   P 21 21 21   R = 0.05   RES=   0   48 X