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: 2a

```
Bond precision:  C-C = 0.0033 A          Wavelength=0.71073

Cell:            a=8.9827(2)     b=23.6098(6)        c=22.1855(5)
                 alpha=90        beta=90.818(1)      gamma=90
Temperature:     193 K
```

	Calculated	Reported
Volume	4704.62(19)	4704.62(19)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C49 H62 I Mg N3 O	?
Sum formula	C49 H62 I Mg N3 O	C49 H62 I Mg N3 O
Mr	860.23	860.23
Dx,g cm-3	1.214	1.215
Z	4	4
Mu (mm-1)	0.730	0.730
F000	1800.0	1800.0
F000'	1798.79	
h,k,lmax	12,32,30	12,32,30
Nref	12871	12780
Tmin,Tmax	0.743,0.775	0.381,0.451
Tmin'	0.616	

```
Correction method= # Reported T Limits: Tmin=0.381 Tmax=0.451
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 29.300

R(reflections)= 0.0363( 7680)     wR2(reflections)= 0.0938( 12780)

S = 0.929                 Npar= 521
```

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

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O53    --  C54     ..       13.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C54    --  C55     ..        8.0 s.u.
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           rod
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT213_ALERT_2_C Atom C443           has ADP max/min Ratio .....        3.7 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        4.5 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C22    --  C221    ..        5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C51    --  C52     ..        6.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C64    --  C65     ..        5.5 s.u.
PLAT245_ALERT_2_C U(iso) H23A    Smaller than U(eq) C23     by ...      0.016 AngSq
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         32 Ang3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.65 mm
PLAT300_ALERT_4_G Atom Site Occupancy of C443    is Constrained at       0.67 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C444    is Constrained at       0.33 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44D    is Constrained at       0.67 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44E    is Constrained at       0.67 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44F    is Constrained at       0.67 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44J    is Constrained at       0.67 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44G    is Constrained at       0.33 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44H    is Constrained at       0.33 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44I    is Constrained at       0.33 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44K    is Constrained at       0.33 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          2 % Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         96 Check
             C444 -C441 -C443    1.555   1.555   1.555            44.10 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
```

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
  13 ALERT type 4 Improvement, methodology, query or suggestion
   1 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

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Publication of your CIF in other journals

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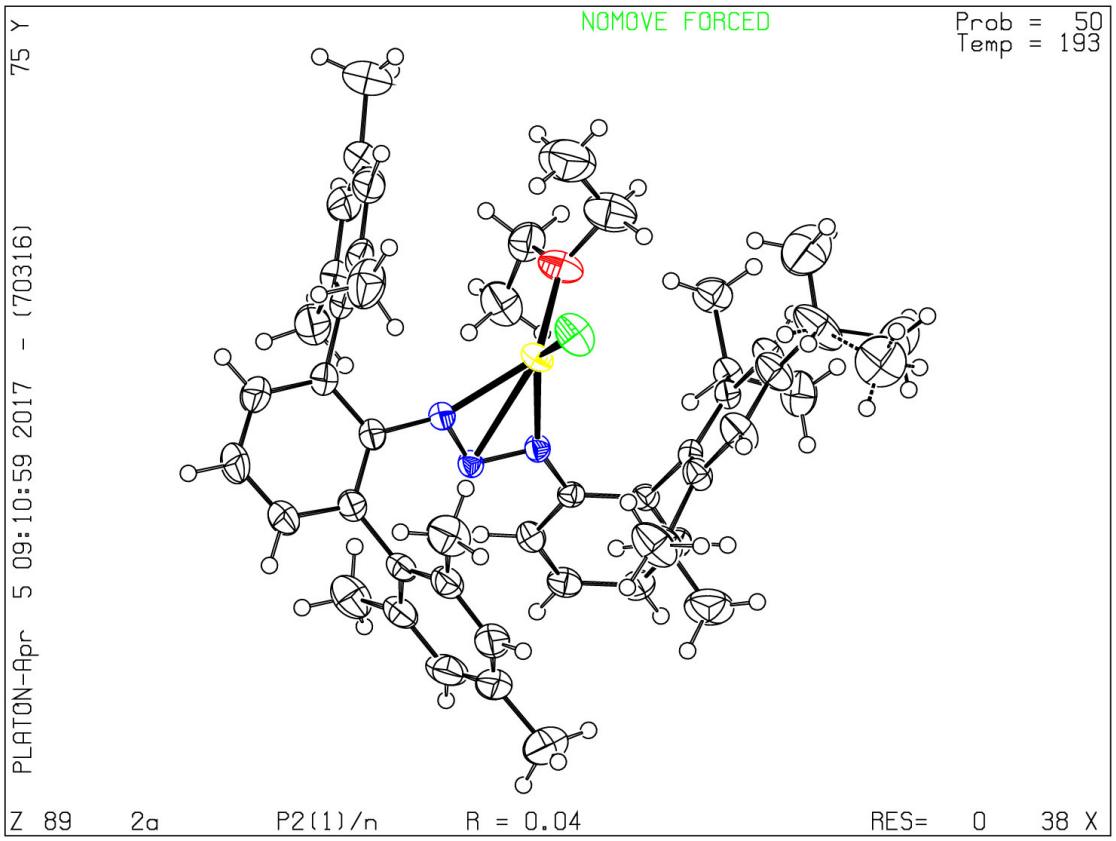
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 2a - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2b

```
Bond precision:  C-C = 0.0038 A          Wavelength=0.71073

Cell:            a=19.848(4)     b=9.373(2)           c=23.033(4)
                 alpha=90        beta=90.386(14)      gamma=90
Temperature:     173 K
```

	Calculated	Reported
Volume	4284.9(15)	4284.9(14)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C48 H52 I Mg N3 O	?
Sum formula	C48 H52 I Mg N3 O	C48 H52 I Mg N3 O
Mr	838.14	838.14
Dx,g cm-3	1.299	1.299
Z	4	4
Mu (mm-1)	0.800	0.800
F000	1736.0	1736.0
F000'	1734.78	
h,k,lmax	25,12,29	25,12,29
Nref	9842	9823
Tmin,Tmax	0.722,0.819	0.533,0.740
Tmin'	0.664	

```
Correction method= # Reported T Limits: Tmin=0.533 Tmax=0.740
AbsCorr = PSI-SCAN

Data completeness= 0.998          Theta(max)= 27.500

R(reflections)= 0.0359( 6945)     wR2(reflections)= 0.0897( 9823)

S = 0.886                 Npar= 501
```

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

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as psi-scan
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
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```

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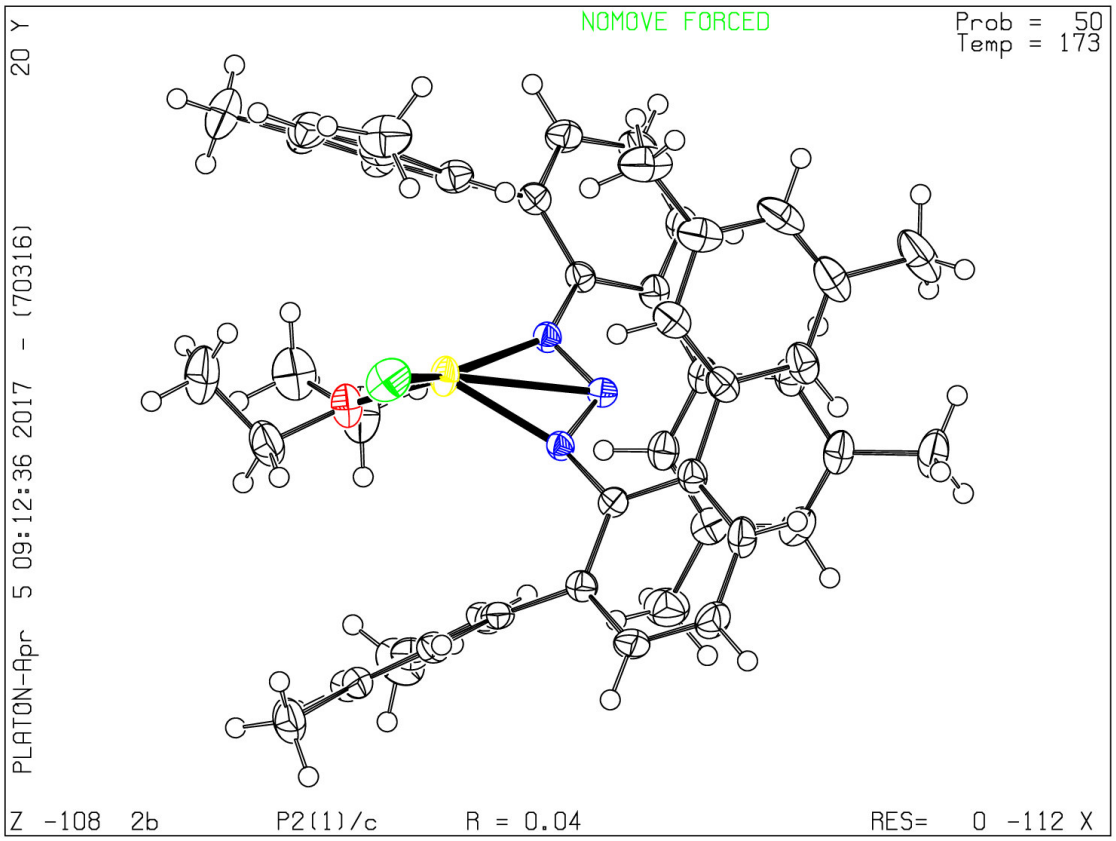
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 2b - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3a

```
Bond precision:  C-C = 0.0088 A          Wavelength=0.71073

Cell:            a=20.4142(4)     b=22.2202(4)     c=39.3523(7)
                 alpha=90         beta=90          gamma=90
Temperature:     173 K

                Calculated                Reported
Volume          17850.5(6)                17850.5(6)
Space group     P b c a                   Pbca
Hall group      -P 2ac 2ab                ?
Moiety formula  C90 H104 I4 Mg3 N6        ?
Sum formula     C90 H104 I4 Mg3 N6        C90 H104 I4 Mg3 N6
Mr              1850.33                   1850.32
Dx,g cm-3       1.377                     1.377
Z               8                         8
Mu (mm-1)       1.462                     1.462
F000            7472.0                    7472.0
F000'           7459.72
h,k,lmax        26,29,51                  26,29,51
Nref            21349                     21302
Tmin,Tmax       0.711,0.803               0.426,0.517
Tmin'           0.639

Correction method= # Reported T Limits: Tmin=0.426 Tmax=0.517
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 27.910

R(reflections)= 0.0411( 6128)     wR2(reflections)= 0.0665( 21302)

S = 0.653                 Npar= 952
```

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.254
PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 29 %

Alert level B

PLAT213_ALERT_2_B Atom C110 has ADP max/min Ratio ..... 4.3 prolat
PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.3 Ratio

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.653
PLAT213_ALERT_2_C Atom C64 has ADP max/min Ratio ..... 3.8 prolat
PLAT213_ALERT_2_C Atom C112 has ADP max/min Ratio ..... 3.1 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 5.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C32 -- C33 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C110 -- C111 .. 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of I1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C64 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C110 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C104 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C107 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C541 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C561 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00881 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C110 - C111 .. 1.37 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C110 - C112 .. 1.37 Ang.

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT020_ALERT_3_G The value of Rint is greater than 0.12 ..... 0.254 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C110 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C721 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C841 Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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5 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
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Publication of your CIF in other journals

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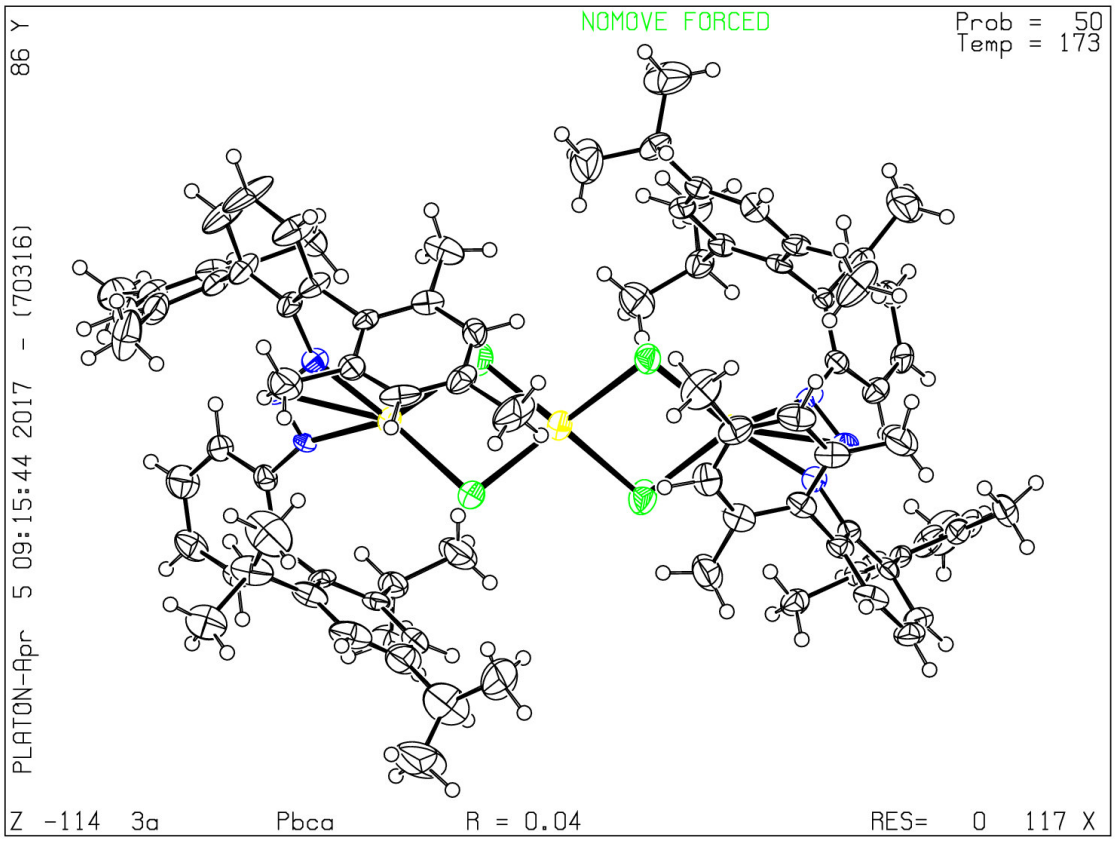
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 3a - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3bheptane

```
Bond precision:  C-C = 0.0071 A          Wavelength=0.71073

Cell:          a=16.9933(5)      b=17.5771(5)     c=17.8005(5)
               alpha=93.427(2)   beta=99.534(2)   gamma=109.991(2)
Temperature:   173 K
```

	Calculated	Reported
Volume	4888.5(3)	4888.5(2)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C88 H84 I4 Mg3 N6	?
Sum formula	C88 H84 I4 Mg3 N6	C88 H84 I4 Mg3 N6
Mr	1806.15	1806.14
Dx,g cm-3	1.227	1.227
Z	2	2
Mu (mm-1)	1.334	1.334
F000	1804.0	1804.0
F000'	1800.93	
h,k,lmax	23,24,24	23,24,24
Nref	27392	27255
Tmin,Tmax	0.577,0.766	0.565,0.823
Tmin'	0.543	

```
Correction method= # Reported T Limits: Tmin=0.565 Tmax=0.823
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 29.550

R(reflections)= 0.0674( 21930)    wR2(reflections)= 0.1344( 27255)

S = 1.921                 Npar= 926
```

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

PLAT213_ALERT_2_A Atom C25 has ADP max/min Ratio ..... 7.8 prolat
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Alert level B

PLAT213_ALERT_2_B Atom C24 has ADP max/min Ratio ..... 4.2 prolat
PLAT213_ALERT_2_B Atom C251 has ADP max/min Ratio ..... 4.9 prolat
PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for C25 -- C26 .. 7.8 s.u.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C24 Check

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT213_ALERT_2_C Atom C23 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C64 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C231 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C651 has ADP max/min Ratio ..... 3.3 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C24 -- C25 .. 7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C113 -- C117 .. 5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 -- C26 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C25 -- C251 .. 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C64 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C65 Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I4 -- Mg2 .. 5.2 s.u.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C21 -C26 0.22 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 3 Do !
N2 -MG1 -MG2 -I1 67.40 0.70 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 7 Do !
N2 -MG1 -MG2 -I2 -113.50 0.70 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 11 Do !
N2 -MG1 -MG2 -I4 -20.70 0.70 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 16 Do !
N2 -MG1 -MG2 -I3 156.50 0.60 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 19 Do !
N3 -MG1 -MG2 -MG3 18.00 0.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 20 Do !
N1 -MG1 -MG2 -MG3 -25.00 4.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 21 Do !
N2 -MG1 -MG2 -MG3 -89.00 3.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 22 Do !
I2 -MG1 -MG2 -MG3 24.00 3.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 23 Do !
I1 -MG1 -MG2 -MG3 -157.00 3.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 28 Do !
MG1 -MG2 -MG3 -N4 -43.00 4.00 1.555 1.555 1.555 1.555

```
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         33 Do !
           MG1 -MG2 -MG3 -N6    127.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         38 Do !
           MG1 -MG2 -MG3 -N5    109.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         42 Do !
           MG1 -MG2 -MG3 -I3   -115.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         46 Do !
           MG1 -MG2 -MG3 -I4     69.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         94 Do !
           MG2 -MG1 -N2  -N3   -104.10  0.70   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         98 Do !
           MG2 -MG1 -N2  -N1     75.10  0.70   1.555   1.555   1.555   1.555
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
   2 ALERT level A = Most likely a serious problem - resolve or explain
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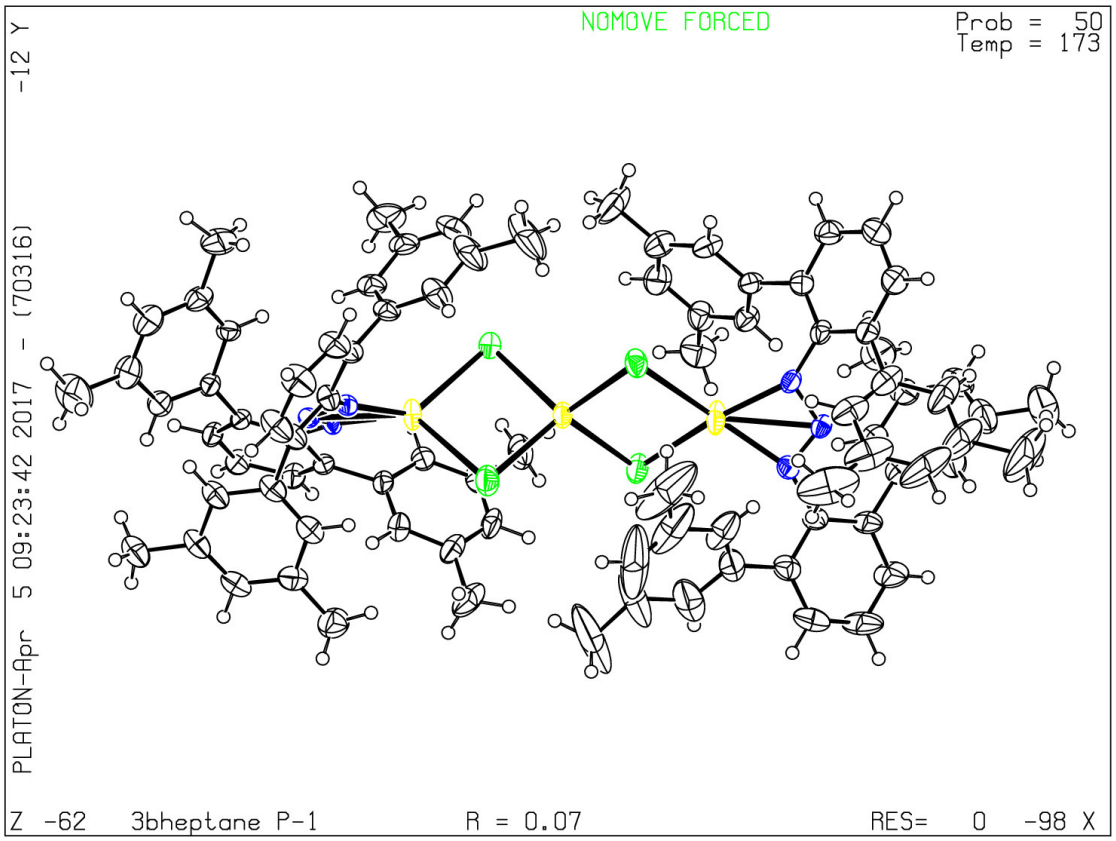
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 3bheptane - ellipsoid plot



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: 4bheptane

```
Bond precision:  C-C = 0.0042 A          Wavelength=0.71073

Cell:           a=15.0589(12)    b=13.0937(10)      c=20.3232(16)
                alpha=90         beta=99.013(3)     gamma=90
Temperature:    173 K

                Calculated                Reported
Volume          3957.8(5)                 3957.8(5)
Space group     P 2/n                     P2/n
Hall group      -P 2yac                   ?
Moiety formula  C88 H84 Mg N6, C7 H16     ?
Sum formula     C95 H100 Mg N6            C47.50 H50 Mg0.50 N3
Mr              1350.12                   675.06
Dx,g cm-3       1.133                     1.133
Z               2                         4
Mu (mm-1)       0.073                     0.073
F000            1448.0                    1448.0
F000'           1448.54
h,k,lmax        19,17,26                  19,17,26
Nref            9097                      9087
Tmin,Tmax       0.978,0.986
Tmin'           0.975

Correction method= Not given

Data completeness= 0.999          Theta(max)= 27.500

R(reflections)= 0.0665( 3669)     wR2(reflections)= 0.1882( 9087)

S = 0.885                 Npar= 464
```

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

```
RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
            Rint given   0.248
```

Alert level C

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..         40 %
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          1 Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1     --  N2      ..        6.0 s.u.
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C204 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00421 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H65B   ..  H65B    ..       2.09 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT020_ALERT_3_G The value of Rint is greater than 0.12 .........      0.248 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT300_ALERT_4_G Atom Site Occupancy of C201    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C202    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C203    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C301    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C302    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C303    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20C    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20D    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20E    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20F    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20G    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20H    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20I    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30A    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30B    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30C    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30D    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30E    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30F    is Constrained at         0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30G    is Constrained at         0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..          86 % Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         100 Check
             C303 -C204 -C203    2.554   1.555   2.554             43.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         103 Check
             C303 -C204 -C203    1.555   1.555   1.555             43.90 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #           2 Note
             C7 H16
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          8 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

---

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

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

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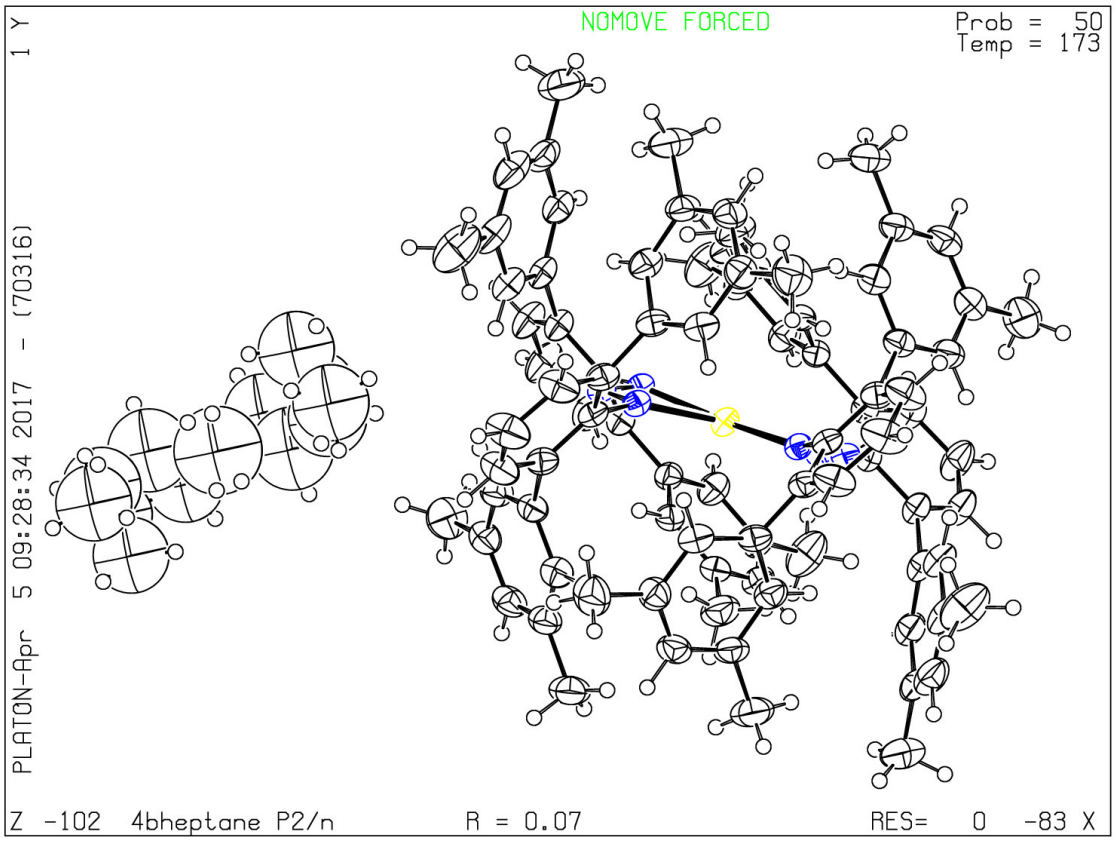
PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 4bheptane - ellipsoid plot



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: 4ctoluene

```
Bond precision:  C-C = 0.0036 A          Wavelength=0.71073

Cell:            a=13.302(2)    b=21.531(3)          c=24.332(4)
                 alpha=90       beta=101.877(12)     gamma=90
Temperature:     173 K
```

	Calculated	Reported
Volume	6819.6(18)	6819.8(17)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	2(C78 H80 Mg N6), C7 H8	?
Sum formula	C163 H168 Mg2 N12	C81.50 H84 Mg N6
Mr	2343.72	1171.86
Dx,g cm-3	1.141	1.141
Z	2	4
Mu (mm-1)	0.075	0.075
F000	2508.0	2508.0
F000'	2508.96	
h,k,lmax	15,25,28	15,25,28
Nref	12012	11996
Tmin,Tmax	0.965,0.978	
Tmin'	0.963	

```
Correction method= Not given

Data completeness= 0.999          Theta(max)= 25.000

R(reflections)= 0.0435( 5484)     wR2(reflections)= 0.0981( 11996)

S = 0.727                 Npar= 837
```

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

```
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.727
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..         46 %
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        3.9 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2   H   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N5     --  N6      ..        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C84    --  C85     ..        6.0 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.8 Note
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C201    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C202    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C203    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C204    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C205    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C206    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C207    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B    is Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H202    is Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of H204    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H205    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H206    is Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..        100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.50) in Resd. #          2 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C841 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C206    ..       1.02 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C205    ..       1.10 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C201    ..       1.39 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C204    ..       1.50 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C202    ..       1.73 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C203    ..       1.78 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C201   ..  C207    ..       2.87 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C206    ..       0.42 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C205    ..       1.50 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C207    ..       2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C204    ..       2.68 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C202    ..       2.82 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C202   ..  C203    ..       3.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C203   ..  C206    ..       1.50 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C203   ..  C207    ..       1.77 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C203   ..  C205    ..       2.87 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C204   ..  C207    ..       0.41 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C204   ..  C206    ..       2.28 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C205   ..  C207    ..       1.11 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C205   ..  C206    ..       2.46 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C206   ..  C206    ..       2.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C206   ..  C207    ..       2.29 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

---

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