checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj220913a

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: hasj220913a

```
Bond precision:   C-C = 0.0046 A          Wavelength=1.54184

Cell:             a=19.4688(3)    b=22.1144(3)         c=45.7469(5)
                  alpha=90        beta=98.7055(12)     gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	19469.0(5)	19469.0(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C43 H69 Mg N2, C12 H36 N2 Na3 Si4	C55 H105 Mg N4 Na3 Si4
Sum formula	C55 H105 Mg N4 Na3 Si4	C55 H105 Mg N4 Na3 Si4
Mr	1028.07	1028.06
Dx,g cm-3	1.052	1.052
Z	12	12
Mu (mm-1)	1.394	1.394
F000	6768.0	6768.0
F000'	6799.23	
h,k,lmax	23,26,54	23,26,54
Nref	34771	34611
Tmin,Tmax	0.627,0.913	0.262,1.000
Tmin'	0.509	

```
Correction method= # Reported T Limits: Tmin=0.262 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.995          Theta(max)= 67.079

R(reflections)= 0.0736( 25418)                    wR2(reflections)=
                                                  0.2166( 34611)
S = 1.022                 Npar= 2241
```

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C43 H69 Mg N2, C12 H36 N2 Na3 Si4
             Rep.: C55 H105 Mg N4 Na3 Si4
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Na9 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Na3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Si10 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00459 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.379 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.597        157 Report
               20  7  0,  16 16  0,  17 16  0,  18 16  0,  16 17  0, -23  0  1,
               17  4  1,  20  4  1,  18  6  1, -18 16  1, -17 16  1, -16 16  1,
               16 16  1,  17 16  1, -16 17  1, -15 17  1,  16 17  1, -18  3  2,
              -17  5  2, -20 11  2, -18 11  2, -18 16  2, -17 16  2, -16 16  2,
               17 16  2, -16 17  2, -15 17  2, -23  0  3, -18  8  3, -18 16  3,
              -17 16  3, -16 16  3, -15 16  3,  17 16  3, -16 17  3, -15 17  3,
              -14 17  3, -17 12  4, -18 16  4, -17 16  4, -16 16  4, -15 16  4,
               17 16  4, -16 17  4, -15 17  4, -14 17  4, -12 22  4, -23  0  5,
              -22  5  5, -21  9  5, -19 15  5, -18 16  5, -17 16  5, -16 17  5,
              -15 17  5, -14 17  5, -13 17  5,  12 22  5, -21  4  6, -20  7  6,
               18 15  6, -18 16  6, -16 17  6, -15 17  6, -14 17  6, -13 17  6,
               17 17  6,  14 20  6,  13 21  6,  11 22  6,  12 22  6, -11 23  6,
               -2 26  6, -23  0  7, -20 11  7, -18 16  7, -16 17  7, -15 17  7,
               16 18  7,  15 19  7,  14 20  7,  12 21  7,  13 21  7,  11 22  7,
              -19 10  8, -20 11  8, -17 14  8,  18 15  8, -18 16  8,  17 16  8,
              -16 17  8,  15 19  8,  14 20  8,  12 21  8,  13 21  8,  11 22  8,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         72 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          68 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      15.55 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          7 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0300 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0020 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        22% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)        11% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        38% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)        43% Note
```

```
PLAT410_ALERT_2_G Short Intra H...H Contact  H14      ..H19A     .       2.08 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H16      ..H26A     .       2.12 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H5A      ..H24A     .       2.07 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H6A      ..H18A     .       2.08 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H7C      ..H24A     .       1.99 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H64A     ..H92B     .       2.09 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H66C     ..H92B     .       2.14 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H99A     ..H17P     .       2.08 Ang.
                                                     x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          7 Note
              H1AA    H1AH    H1AI    H1AF    H1AG    H1AB    H1AC
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............       2305 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        61% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               -1  0  1,   0  1  1,   0  0  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.018 Note
              Predicted wR2: Based on SigI**2  7.18 or SHELX Weight 21.20
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
```

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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
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
36 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
18 ALERT type 2 Indicator that the structure model may be wrong or deficient
18 ALERT type 3 Indicator that the structure quality may be low
6 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

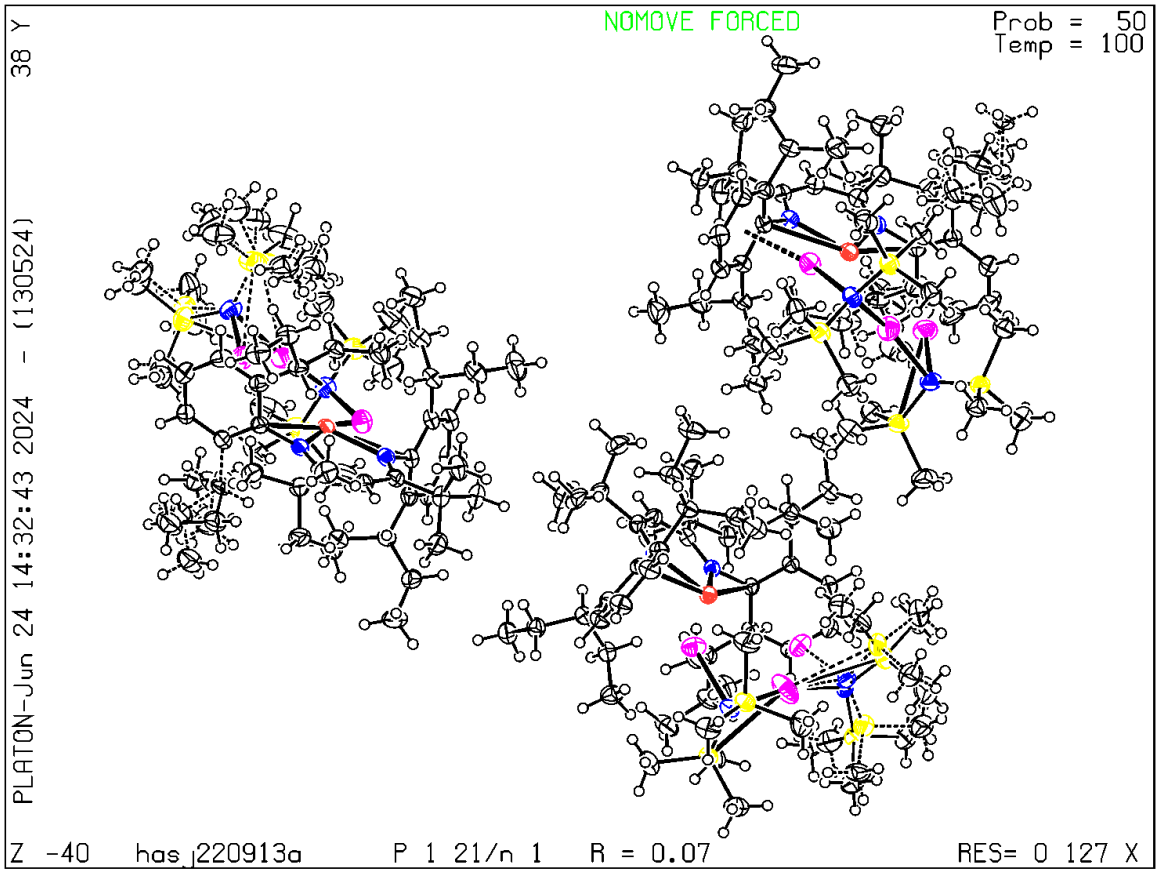
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/05/2024; check.def file version of 04/05/2024

Datablock hasj220913a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj220919a

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: hasj220919a

```
Bond precision:   C-C = 0.0059 A          Wavelength=1.54184

Cell:             a=20.4668(2)      b=14.4504(2)      c=21.7229(3)
                  alpha=90          beta=90           gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           6424.62(14)                 6424.62(14)
Space group      P c a 21                    P c a 21
Hall group       P 2c -2ac                   P 2c -2ac
Moiety formula   C55 H105 Mg N4 Na3 O Si4    C55 H105 Mg N4 Na3 O Si4
Sum formula      C55 H105 Mg N4 Na3 O Si4    C55 H105 Mg N4 Na3 O Si4
Mr               1044.07                     1044.06
Dx,g cm-3        1.079                       1.079
Z                4                           4
Mu (mm-1)        1.427                       1.427
F000             2288.0                      2288.0
F000'            2298.61
h,k,lmax         25,17,26                    25,17,26
Nref             12765[ 6563]                10974
Tmin,Tmax        0.850,0.895                 0.841,1.000
Tmin'            0.806

Correction method= # Reported T Limits: Tmin=0.841 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.67/0.86        Theta(max)= 72.695

R(reflections)= 0.0432( 10231)                wR2(reflections)=
                                              0.1189( 10974)
S = 1.038                  Npar= 778
```

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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.13 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.1 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si2 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0059 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          4 Report
              11 15  0,  12 15  0,   0  3  4,  12 10 17,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         28 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          17 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C21      --C22      .        6.8 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        21% Note
PLAT303_ALERT_2_G Full Occupancy Atom H42B      with # Connections       2.00 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H14      ..H21B     .       2.14 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H14      ..H21D     .       2.14 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H19A     ..H21C     .       2.13 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H18      ..H22F     .       1.90 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H49A     ..H46F     .       1.91 Ang.
                                             x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C22      ..C41      .       3.16 Ang.
                                          1-x,-y,-1/2+z  =      2_654 Check
PLAT792_ALERT_1_G Model has Chirality at C18         (Polar  SpGr)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        762 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        102 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         73 %
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
              10 13 11,  18  6-14,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.468 Note
             Predicted wR2: Based on SigI**2  3.43 or SHELX Weight 11.45
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

---

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
22 **ALERT level G** = General information/check it is not something unexpected

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

```
 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  3 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

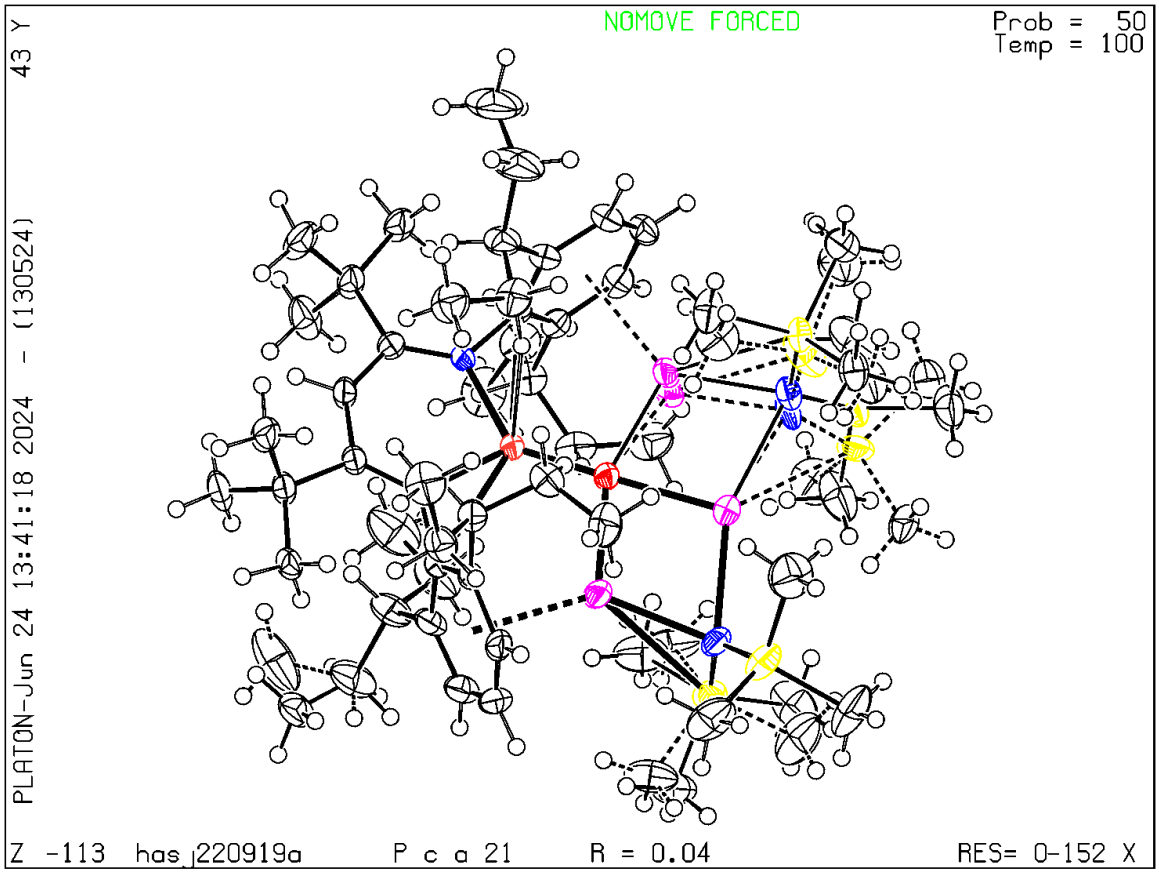
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/05/2024; check.def file version of 04/05/2024

Datablock hasj220919a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj220203b

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: hasj220203b

Bond precision: C-C = 0.0024 A Wavelength=1.54184

Cell: a=12.1701(4) b=12.4334(3) c=18.6675(5)
alpha=79.887(2) beta=75.914(3) gamma=63.312(3)
Temperature: 100 K

	Calculated	Reported
Volume	2440.70(14)	2440.70(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C86 H138 Mg2 N4 Na2 O2, 3(C7 H8)	C86 H138 Mg2 N4 Na2 O2, 3(C7 H8)
Sum formula	C107 H162 Mg2 N4 Na2 O2	C107 H162 Mg2 N4 Na2 O2
Mr	1631.01	1631.00
Dx,g cm-3	1.110	1.110
Z	1	1
Mu (mm-1)	0.677	0.677
F000	894.0	894.0
F000'	896.62	
h,k,lmax	15,15,23	15,15,23
Nref	9693	9409
Tmin,Tmax	0.854,0.936	0.713,1.000
Tmin'	0.825	

Correction method= # Reported T Limits: Tmin=0.713 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.971 Theta(max)= 72.668

R(reflections)= 0.0473(8401) wR2(reflections)= 0.1335(9409)

S = 1.034 Npar= 626

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 NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C44      0.110 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         41 Report
               13 11  0, -12-12  1, -10-13  2, -11-12  2, -12-11  2, -10-13  3,
              -11-12  3, -12-11  3, -11-11  3, -11-11  4,  12 -2  4,  13  0  4,
               14 10  4,  12 -2  5,  13  0  5,  14 10  5,  11 -3  6,  11 -2  6,
               14 10  6,  14 10  7,  14  9  8,  14  9  9,  14  9 10,   5 14 10,
               13  8 11,  14  8 11,  13  9 11,  13 10 11,  13 11 11,   6 14 11,
               13  8 12,  13  9 12,  13 10 12,  13  8 13,  13  9 13,  12 10 13,
               12 11 13,  13  7 14,  13  8 14,  12 10 14,  -1 -1 21,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         9 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms         21 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0020 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0020 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0100 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C53      --C54      .        6.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C44        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C46        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C47        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C48        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C49        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C50        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H45        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H46        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H47        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H48        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H49        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H50C       Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        100% Note
PLAT303_ALERT_2_G Full Occupancy Atom H1        with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H20A      with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H20B      with # Connections       2.00 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       7.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)      11.55 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       3.45 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for        C20 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C19      - C20      .       1.55 Ang.
```

```
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H7C      ..H57D     .       1.84 Ang.
                                                -x,1-y,1-z  =      2_566 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H9A      ..H57D     .       2.03 Ang.
                                                -x,1-y,1-z  =      2_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7       ..C57A     .       3.19 Ang.
                                                -x,1-y,1-z  =      2_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C9       ..C57A     .       3.18 Ang.
                                                -x,1-y,1-z  =      2_566 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      44.29 Deg.
             N1   -C12  -MG1     1_555   1_555   1_555 ......     #  101 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         15 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        651 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
               0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        241 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.632 Note
             Predicted wR2: Based on SigI**2  3.66 or SHELX Weight 12.92
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         12 Info
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
50 **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
9 ALERT type 3 Indicator that the structure quality may be low
29 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.

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Publication of your CIF in other journals

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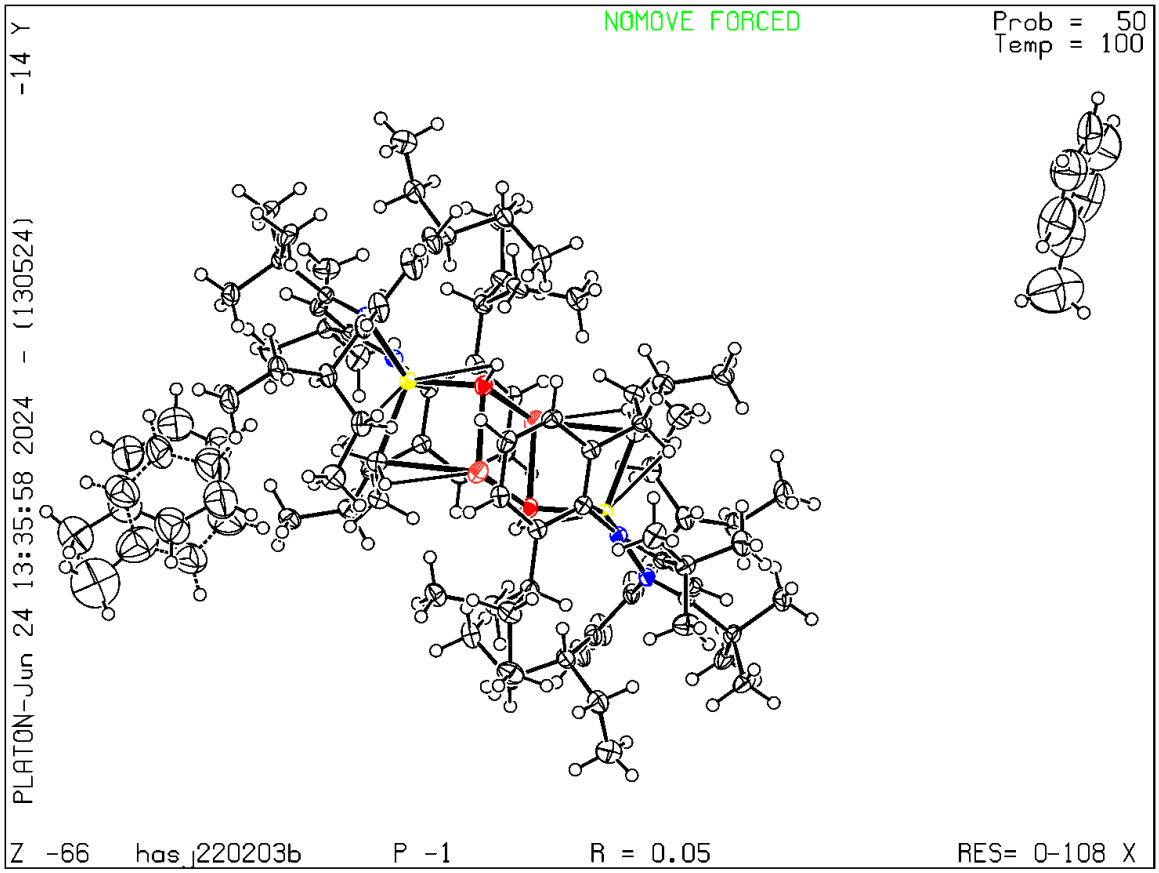
PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock hasj220203b - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj231016a

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: hasj231016a

```
Bond precision:   C-C = 0.0029 A           Wavelength=1.54184

Cell:           a=16.1046(3)       b=19.7957(3)      c=31.4472(4)
                alpha=77.931(1)    beta=86.206(1)    gamma=81.731(1)
Temperature:    100 K
```

	Calculated	Reported
Volume	9695.2(3)	9695.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C55 H105 Mg N4 Na3 O2 Si4	C55 H105 Mg N4 Na3 O2 Si4
Sum formula	C55 H105 Mg N4 Na3 O2 Si4	C55 H105 Mg N4 Na3 O2 Si4
Mr	1060.07	1060.06
Dx,g cm-3	1.089	1.089
Z	6	6
Mu (mm-1)	1.437	1.437
F000	3480.0	3480.0
F000'	3496.20	
h,k,lmax	19,24,38	19,24,38
Nref	38466	37195
Tmin,Tmax	0.750,0.885	0.333,1.000
Tmin'	0.588	

```
Correction method= # Reported T Limits: Tmin=0.333 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.967            Theta(max)= 72.515

R(reflections)= 0.0412( 31634)                    wR2(reflections)=
                                                  0.1045( 37195)
S = 1.042                  Npar= 1942
```

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 NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range         3.2 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 3  C   Ueq(max)/Ueq(min) Range         3.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 3  H   Uiso(max)/Uiso(min) Range         4.2 Ratio
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H        ..H        .        2.13 Ang.
                                                1-x,1-y,1-z  =      2_666 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.920 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        153 Report
              -17  7  0,   2 23  0,   3 23  0,  -4-23  1,  -3-23  1,  -2-23  1,
               12-13  1,   9-12  1,   7 11  1,   4 12  1,   5 12  1,   1 13  1,
                3 13  1,   2 23  1,   3 23  1,   9-12  2,  17 -4  2, -17  7  2,
                8 10  2,   6 11  2,   7 11  2,   5 12  2,   6 12  2,   0 13  2,
                2 23  2,   3 23  2,   1  2  3,  18  4  3,   9  9  3,   8 10  3,
                7 11  3,   6 12  3,  17 14  3,   2 23  3,   3 23  3,   1  3  4,
               19  6  4,  -1 13  4,  17 14  4,   2 23  4,   3 23  4,  -3-22  5,
                1  3  5,   2  3  5,   1  4  5,   2 23  5,   3 23  5,  -4-22  6,
               -3-22  6,  16 -9  6,   2 -2  6,   2  3  6,   1  4  6,   2  4  6,
                1  5  6,  -3 12  6,  16 16  6,   2 23  6,   3 23  6,   1  4  7,
                2  4  7,  -3 12  7,  16 16  7,  15 17  7,   2 23  7,   3 23  7,
               -6-21  8,  10  4  8,   2 23  8,  -3-21  9,   9  4  9,  10  4  9,
               -4 11  9,  -3-21 10,   9  3 11,   9  2 12,   8  3 12,   9  3 12,
               12 12 12,  11 21 12,  -1-20 13,   8  2 13,  11 12 13,  -5  8 14,
                9 22 14,   0-19 15,   1-19 15,  12 -4 15,   8  1 15,   1-18 16,
              -10 17 16,  -9 18 16,   1-18 17,   2-18 17,  -5  5 17, -10 16 17,
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         7 Note
              H1AA    H1AB    H1AC    H1AD    H1AE    H1AF    H1AG
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
                0  1  0,   0  0  1,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1115 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         7 Note
              -17  7  0, -17  7  2,   2 -2  6,  12 -2 28,  17 -4  2,  18  4  3,
               19  6  4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        1.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..........      2.028 Note
              Predicted wR2: Based on SigI**2  5.16 or SHELX Weight 10.03
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         4 Info
```

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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
8 **ALERT level G** = General information/check it is not something unexpected

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

```
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 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
```

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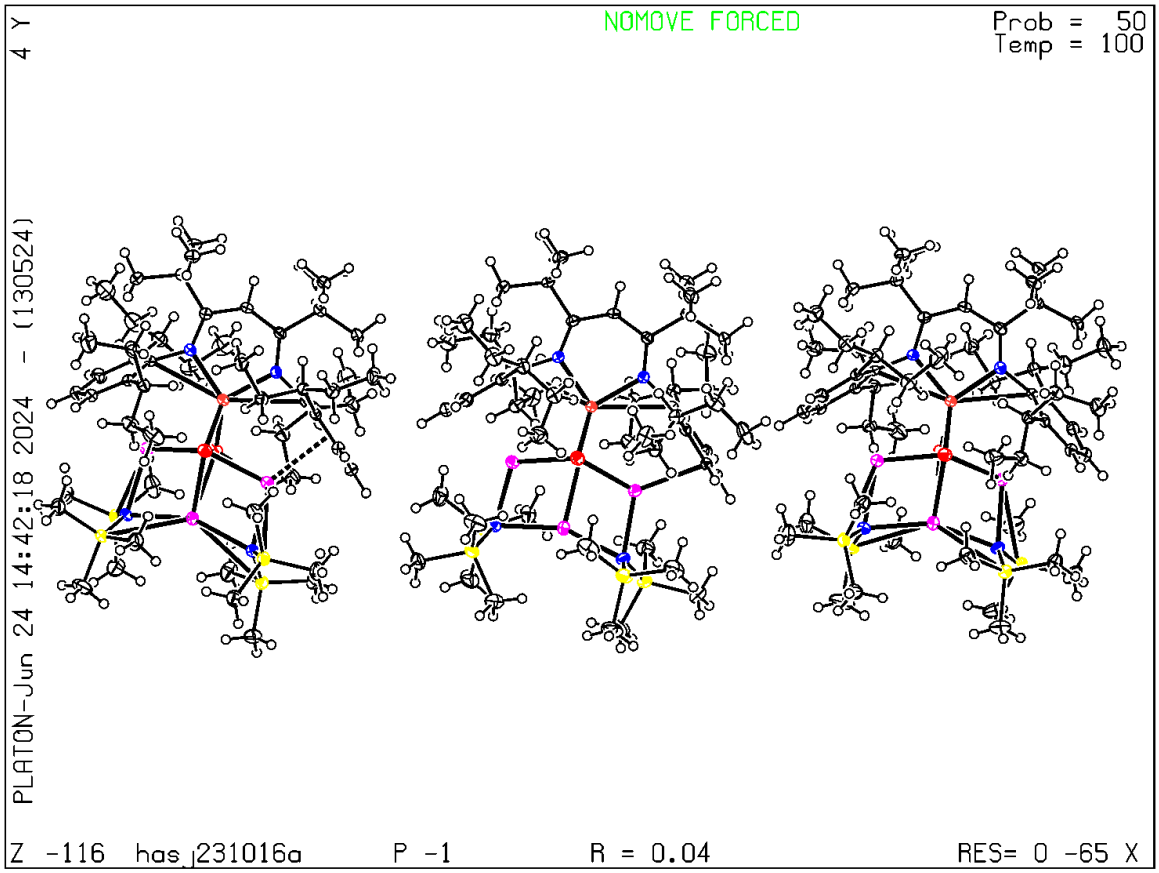
PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock hasj231016a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj230109a

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: hasj230109a

```
Bond precision:   C-C = 0.0022 A          Wavelength=1.54184

Cell:           a=12.32731(12)    b=28.2360(3)       c=22.09076(18)
                alpha=90          beta=97.3103(9)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          7626.72(13)               7626.72(12)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C61 H123 Mg N7 Na4 O2 Si6 C61 H123 Mg N7 Na4 O2 Si6
Sum formula     C61 H123 Mg N7 Na4 O2 Si6 C61 H123 Mg N7 Na4 O2 Si6
Mr              1271.48                   1271.47
Dx,g cm-3       1.107                     1.107
Z               4                         4
Mu (mm-1)       1.645                     1.645
F000            2776.0                    2776.0
F000'           2790.06
h,k,lmax        15,34,27                  14,34,26
Nref            14957                     14412
Tmin,Tmax       0.756,0.828               0.769,1.000
Tmin'           0.685

Correction method= # Reported T Limits: Tmin=0.769 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.964          Theta(max)= 71.874

R(reflections)= 0.0387( 12385)                wR2(reflections)=
                                              0.1073( 14412)
S = 1.017                 Npar= 848
```

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

```
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem         C          95 %Fit
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si2      --C49      .        5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si3      --C51      .        5.6 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si3 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        70 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         21 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         19 Report
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00018 Ang.
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          5 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0030 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0030 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mg1      --O2       .        5.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        11% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H16      ..H26B     .       2.10 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H32      ..H40D     .       2.04 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H16      ..H27D     .       2.09 Ang.
                                                     x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H32      ..H41C     .       2.07 Ang.
                                                     x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H50B     ..H26D     .       2.11 Ang.
                                                  -x,1/2+y,1/2-z  =      2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C30      ..C41A     .       3.07 Ang.
                                                     1-x,1-y,1-z  =      3_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C31      ..C41A     .       2.92 Ang.
                                                     1-x,1-y,1-z  =      3_666 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        597 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        424 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         10 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

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

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

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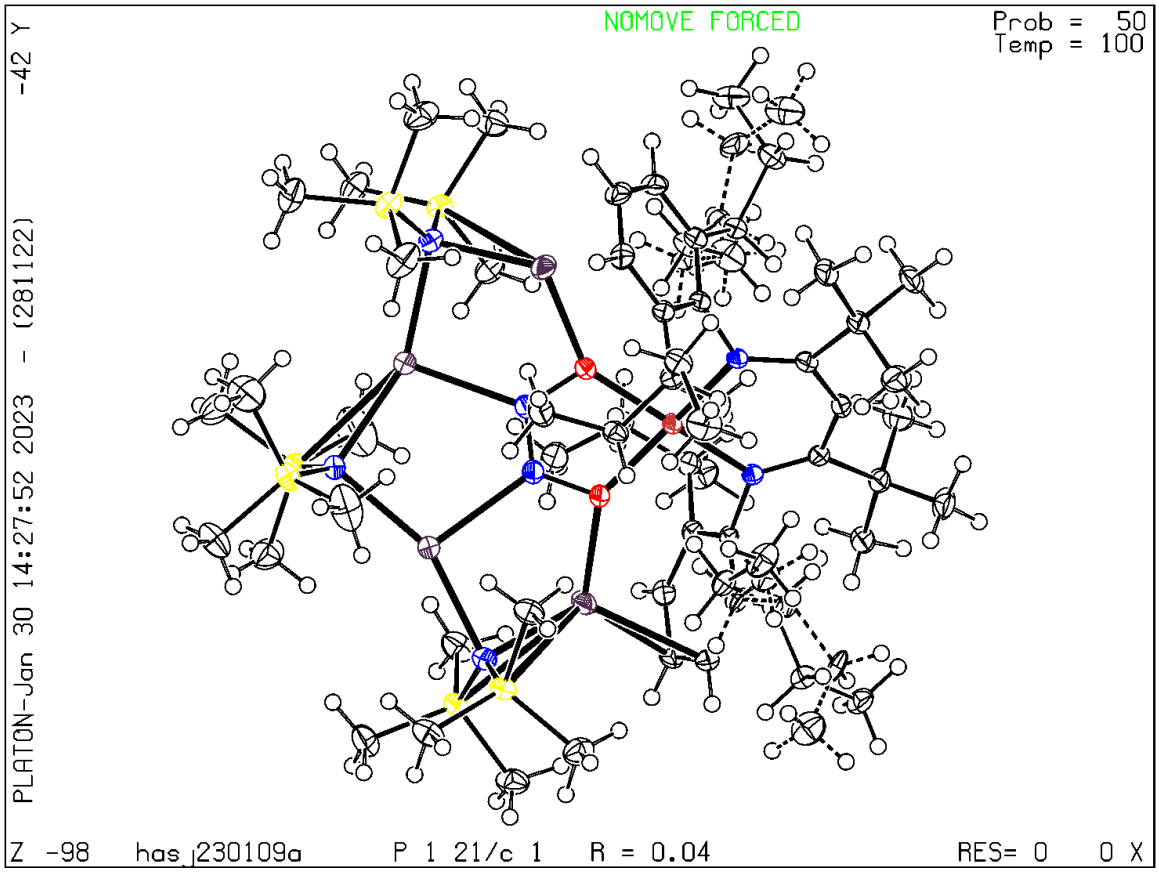
PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock hasj230109a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj240220a

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: hasj240220a

```
Bond precision:   C-C = 0.0017 A          Wavelength=1.54184

Cell:             a=10.3537(1)     b=19.5644(2)        c=21.7614(2)
                  alpha=90         beta=96.920(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           4375.96(7)                4375.96(7)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C47 H77 N2 Na O           C47 H77 N2 Na O
Sum formula      C47 H77 N2 Na O           C47 H77 N2 Na O
Mr               709.10                    709.09
Dx,g cm-3        1.076                     1.076
Z                4                         4
Mu (mm-1)        0.554                     0.554
F000             1568.0                    1568.0
F000'            1572.15
h,k,lmax         12,24,26                  12,23,26
Nref             8692                      8426
Tmin,Tmax        0.865,0.903               0.582,1.000
Tmin'            0.804

Correction method= # Reported T Limits: Tmin=0.582 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.969           Theta(max)= 72.578

R(reflections)= 0.0367( 7571)                wR2(reflections)=
                                             0.0950( 8426)
S = 1.025                 Npar= 520
```

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 NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range         3.3 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          20 Report
                  0 12  0,   1 13  0,   1  0  1,   1 12  1,   0 13  1,   1 13  1,
                  2  0  2,   1 12  2,   0 13  2,   2 23  2,   2 12  3,  -6  0  6,
                 -6  1  6,   2 22  7,  -5  0 11,  -4  0 12,   3 18 14, -10  0 16,
                 -6  0 22,  -3 12 22,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          10 Report
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00020 Ang.
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        10% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        224 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                  0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        235 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.667 Note
             Predicted wR2: Based on SigI**2  3.56 or SHELX Weight  9.27
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         19 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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```

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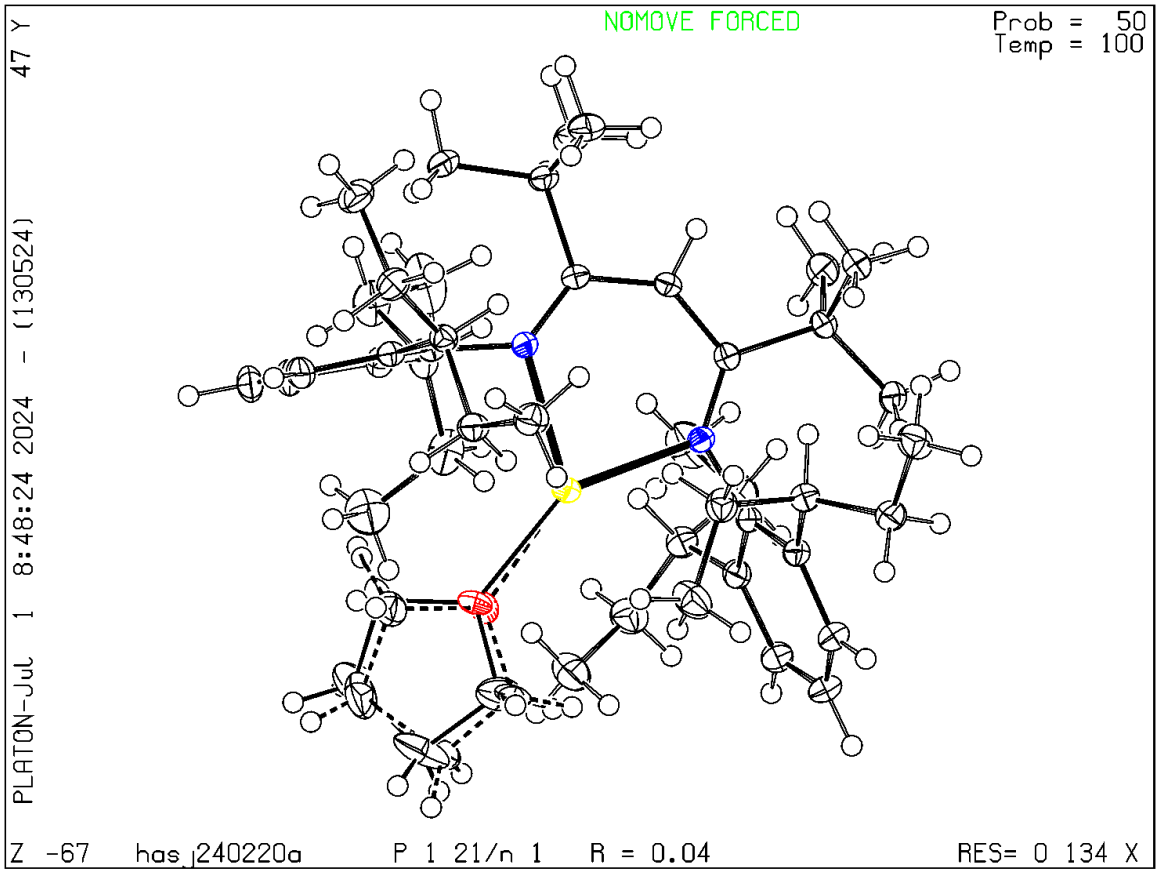
Publication of your CIF in other journals

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

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock hasj240220a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hasj211112a

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: hasj211112a

Bond precision: C-C = 0.0025 A Wavelength=1.54184

Cell: a=11.4384(3) b=15.0170(3) c=36.1820(7)
alpha=82.6283(16) beta=85.6640(17) gamma=70.183(2)
Temperature: 100 K

	Calculated	Reported
Volume	5795.2(2)	5795.2(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C55 H93 N2 Na O3), C6 H14, 0.5(C6 H6)	1(C55 H93 N2 Na O3), 0.5(C6 H14), 0.25(C6 H6)
Sum formula	C119 H203 N4 Na2 O6	C59.50 H101.50 N2 Na O3
Mr	1831.83	915.91
Dx,g cm-3	1.050	1.050
Z	2	4
Mu (mm-1)	0.539	0.539
F000	2030.0	2030.0
F000'	2035.40	
h,k,lmax	14,18,44	14,18,44
Nref	23028	22211
Tmin,Tmax	0.852,0.900	0.431,1.000
Tmin'	0.810	

Correction method= # Reported T Limits: Tmin=0.431 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.965 Theta(max)= 72.690

R(reflections)= 0.0546(18996) wR2(reflections)= 0.1577(22211)

S = 1.017 Npar= 1756

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C55 H93 N2 Na O3), C6 H14, 0.5(C6 H6)
             Rep.: 1(C55 H93 N2 Na O3), 0.5(C6 H14), 0.25(C6 H6)
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    4)        3.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    5)        2.8 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      C117      0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      C140      0.147 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.943 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         90 Report
                  5 16  1,   7  7  2,   7  7  3,  -6 -6  4,  -1  0  5,   1  1  5,
                  7 17  6,   6  5  7,   7 17  7,   2  2  8,   5  4  8,   6  5  8,
                  7 17  8,   2-15  9, -13 -3  9,   5  4  9,   6  5  9,   7 17  9,
                  6  6 10,   8 17 10,   7  2 11,   4  4 11,   5  5 11,   6  6 11,
                  7  3 12,   6  7 12,   4  5 13,   5  6 13,   6  7 13,   6  1 14,
                 -10-13 15,   6  1 15,   5  7 15,  -8  9 15,   6  1 16,  -3  5 16,
                  -2  6 16,  13  8 16,   8 16 16,   8 16 17,  -9-12 18,  -7 10 18,
                   8 16 18,  -8  8 19,  -7  9 19,   8 16 19,  -8  8 20,  -7  9 20,
                   8 16 20,  -7  9 21,   8 15 21,  -7  9 22,  -6 10 22,   8 15 22,
                  -6 10 23,   8 15 23,   8 15 24,  -6  9 25,  -5 10 25,  -6  9 26,
                  -5 10 26,   7 15 26,  -7-11 27,  -5 10 27,  -4-12 28,  -6-11 28,
                  -4 10 28,  -5-11 29,  -4-11 29,  -4-10 29,  -3-10 29,  -2 -9 29,
                  -4 10 29,  -4-10 30,  -3-10 30,  -2 -9 30,  -5  9 30,  -4 10 30,
                  -3 10 31,  -4  9 32,  -3 10 32,  -3  9 33,  -3 10 33,  -3  9 34,
                  -5  0 39,   4  4 41,   5  5 41,   4  3 42,   4  4 42,   4  5 42,
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       92 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms        105 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.500 Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        8 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =        3 Note
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0300 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0200 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par    0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar    0.0010 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O4       --C102     .       7.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C81      --C82      .       6.5 s.u.
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PLAT230_ALERT_2_G Hirshfeld Test Diff for    C107     --C108     .        6.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C115     --C116     .        7.5 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C115     --C139     .        5.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)        77% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        83% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       3.34 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       2.66 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H71      ..H81D     .       2.02 Ang.
                                                    x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H61C     ..H90C     .       1.74 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H62B     ..H141     .       1.98 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H62B     ..H142     .       1.44 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H62C     ..H141     .       1.77 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C60      ..C141     .       3.19 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C62      ..C141     .       2.85 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C62      ..C142     .       2.94 Ang.
                                                 1-x,2-y,2-z  =      2_677 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         24 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       3651 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                0  0  1,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        723 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               -1  0  5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.7 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.649 Note
             Predicted wR2: Based on SigI**2  3.39 or SHELX Weight 15.50
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          8 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          3 Check
```

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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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  47 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 ALERT type 2 Indicator that the structure model may be wrong or deficient
  18 ALERT type 3 Indicator that the structure quality may be low
  14 ALERT type 4 Improvement, methodology, query or suggestion
   3 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

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Datablock hasj211112a - ellipsoid plot