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: compound_1

```
Bond precision:  C-C = 0.0032 A          Wavelength=0.71075

Cell:           a=18.7343(17)    b=11.6636(8)       c=23.2790(18)
                alpha=90         beta=106.937(2)    gamma=90
Temperature:    173 K

                Calculated                Reported
Volume          4866.1(7)                 4866.0(7)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C53 H64 Mg N2 P2          C53 H64 Mg N2 P2
Sum formula     C53 H64 Mg N2 P2          C53 H64 Mg N2 P2
Mr              815.31                    815.35
Dx,g cm-3       1.113                     1.113
Z               4                         4
Mu (mm-1)       0.138                     0.138
F000            1752.0                    1752.0
F000'           1753.48
h,k,lmax        22,14,28                  22,14,28
Nref            8947                      8919
Tmin,Tmax       0.975,0.981               0.897,0.981
Tmin'           0.975

Correction method= # Reported T Limits: Tmin=0.897 Tmax=0.981
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.384

R(reflections)= 0.0406( 7582)     wR2(reflections)= 0.1149( 8919)

S = 1.022                 Npar= 532
```

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

PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 9.5 Ratio

Alert level C

PLAT213_ALERT_2_C Atom C53 has ADP max/min Ratio ..... 3.2 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 9.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C50 -- C51 .. 7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C52 -- C53 .. 0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C44 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C51 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mg1 -- C50 .. 5.7 s.u.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 7 Check
N1 -P1 -MG1 1.555 1.555 1.555 33.91 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 17 Check
N2 -P2 -MG1 1.555 1.555 1.555 32.08 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 18 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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

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

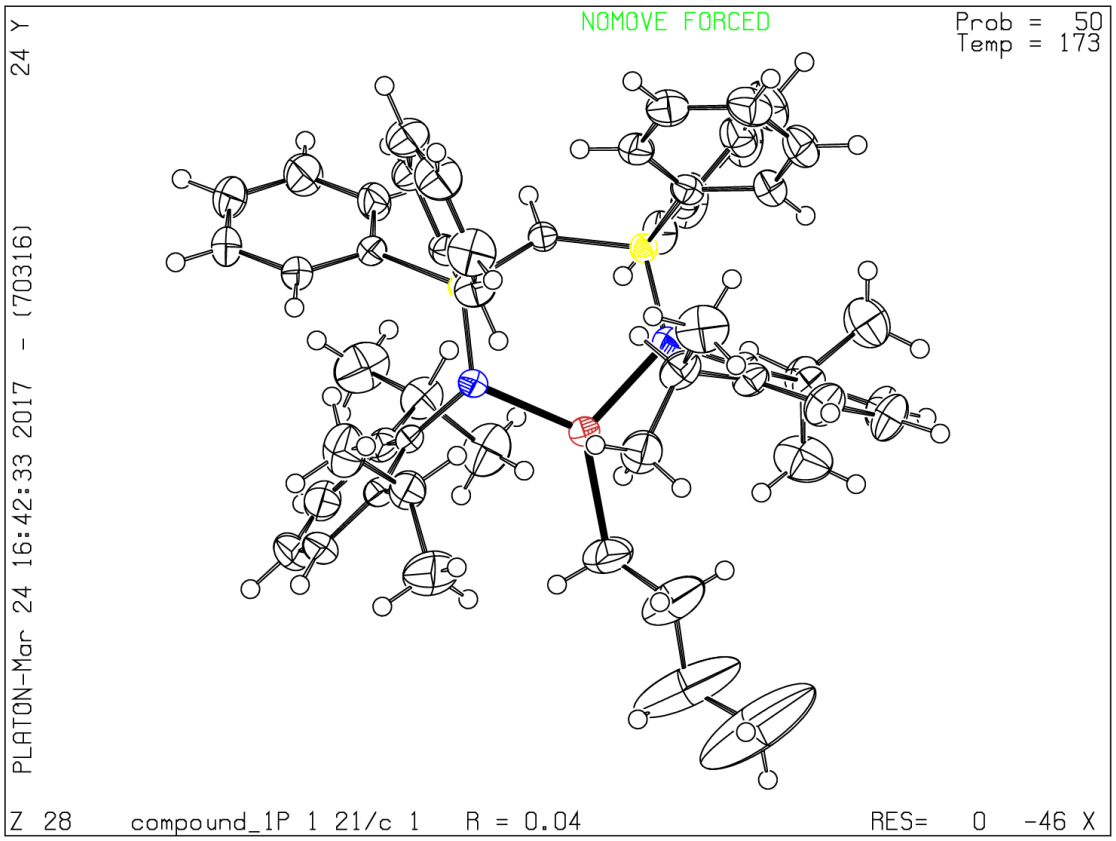
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 26/02/2017; check.def file version of 21/02/2017

Datablock compound_1 - ellipsoid plot



checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_2'

Bond precision: C-C = 0.0031 A Wavelength=0.71070

Cell: a=20.547(4) b=22.500(5) c=22.000(4)
alpha=90 beta=90.34(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	10171(4)	10171(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C98 H108 Mg2 N4 P4, 4(C6 H6)	?
Sum formula	C122 H132 Mg2 N4 P4	C122 H132 Mg2 N4 P4
Mr	1826.82	1826.81
Dx,g cm-3	1.193	1.193
Z	4	4
Mu (mm-1)	0.137	0.139
F000	3904.0	3904.0
F000'	3907.05	
h,k,lmax	27,30,29	27,29,28
Nref	13057	12842
Tmin,Tmax	0.990,0.994	0.990,0.994
Tmin'	0.990	

Correction method= # Reported T Limits: Tmin=0.990 Tmax=0.994
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 28.622

R(reflections)= 0.0554(9091) wR2(reflections)= 0.1406(12842)

S = 1.020 Npar= 713

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

PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor .... 4.9 Note

---

Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT410_ALERT_2_C Short Intra H...H Contact H25 .. H25 . 1.90 Ang.

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 24 Note
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum found in CIF ..... Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.27 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 8 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 8 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 4 Report
PLAT300_ALERT_4_G Atom Site Occupancy of *C50 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C51 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C52 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C53 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C54 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C55 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H50 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H51 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H52 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H53 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H54 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H55 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C60 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C61 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C62 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C63 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C64 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C65 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H60 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H61 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H62 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H63 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H64 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H65 is 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5).. 100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (6.44) in Resd. # 4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (5.56) in Resd. # 5 Check
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C1 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 24 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 60 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
PLAT984_ALERT_1_G The Mg-f'= 0.049 Deviates from the B&C-Value 0.050 Check

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

  4 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
  1 ALERT type 3 Indicator that the structure quality may be low
 34 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

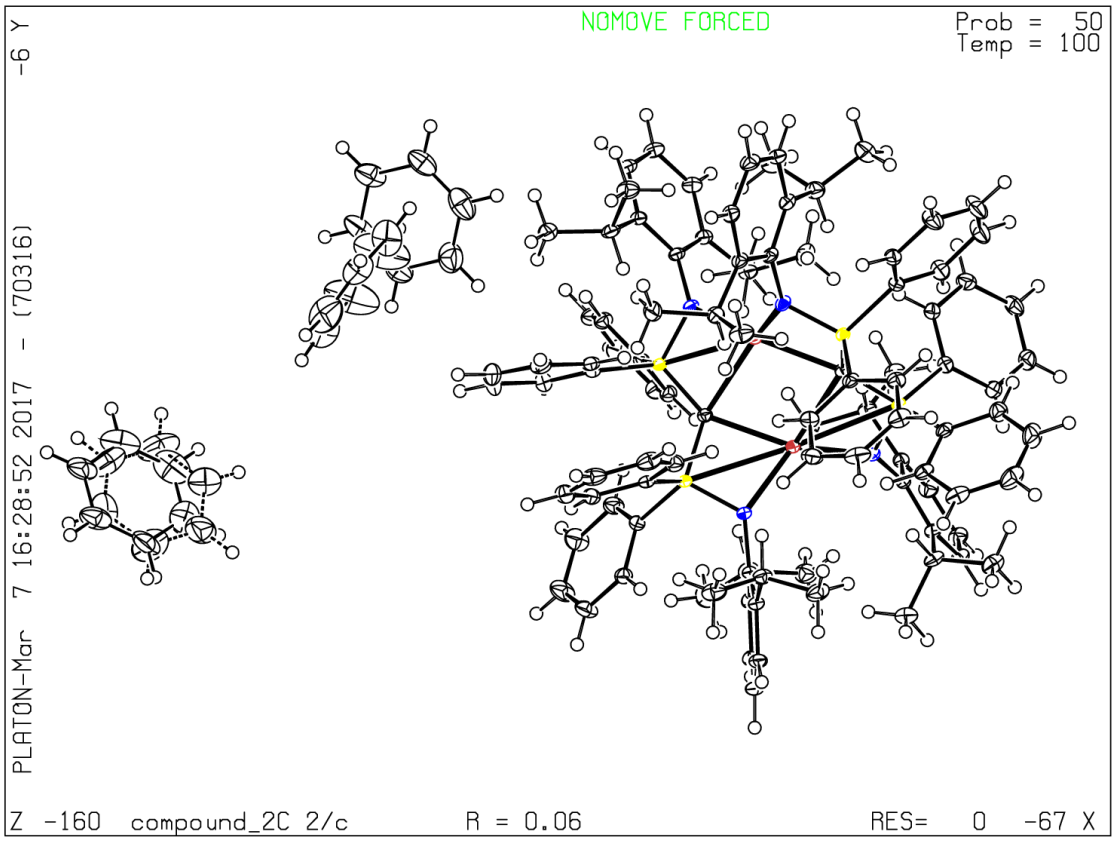
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 26/02/2017; check.def file version of 21/02/2017

Datablock compound_2' - ellipsoid plot



checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_2''

Bond precision: C-C = 0.0023 A Wavelength=0.71080

Cell: a=19.080(4) b=34.382(7) c=16.790(3)
alpha=90 beta=90.56(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	11014(4)	11014(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C98 H108 Mg2 N4 P4, 2(C6 H6) [+ solvent]	?
Sum formula	C110 H120 Mg2 N4 P4 [+ solvent]	C134 H144 Mg2 N4 P4
Mr	1670.60	1983.02
Dx,g cm-3	1.008	1.196
Z	4	4
Mu (mm-1)	0.121	0.134
F000	3568.0	4240.0
F000'	3570.94	
h,k,lmax	24,44,21	24,44,21
Nref	12195	12142
Tmin,Tmax	0.994,0.996	0.991,0.994
Tmin'	0.992	

Correction method= # Reported T Limits: Tmin=0.991 Tmax=0.994
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.138

R(reflections)= 0.0445(10918) wR2(reflections)= 0.1184(12142)

S = 1.051 Npar= 549

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 1983.02
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	110.00	1321.21
H	1.01	120.00	120.96
N	14.01	4.00	56.03
Mg	24.31	2.00	48.61
P	30.97	4.00	123.90

Calculated formula weight 1670.70

Alert level B

PLAT990_ALERT_1_B Deprecated RES file style based SQUEEZE job .... ! Note

---

Alert level C

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C55 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H15 .. H15 . 1.90 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C134 H144 Mg2 N4 P4
Atom count from the _atom_site data: C110 H120 Mg2 N4 P4
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C134 H144 Mg2 N4 P4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	536.00	440.00	96.00
H	576.00	480.00	96.00
Mg	8.00	8.00	0.00
N	16.00	16.00	0.00
P	16.00	16.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum found in CIF ..... Please Check
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum found in CIF ..... Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 15.98 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C1 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 7 Check

```
             N1   -P1   -MG1     1.555   1.555   1.555            44.95 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 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 ...         10 Note
PLAT984_ALERT_1_G The Mg-f'=     0.049 Deviates from the B&C-Value      0.050 Check
```

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

 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 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
  5 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

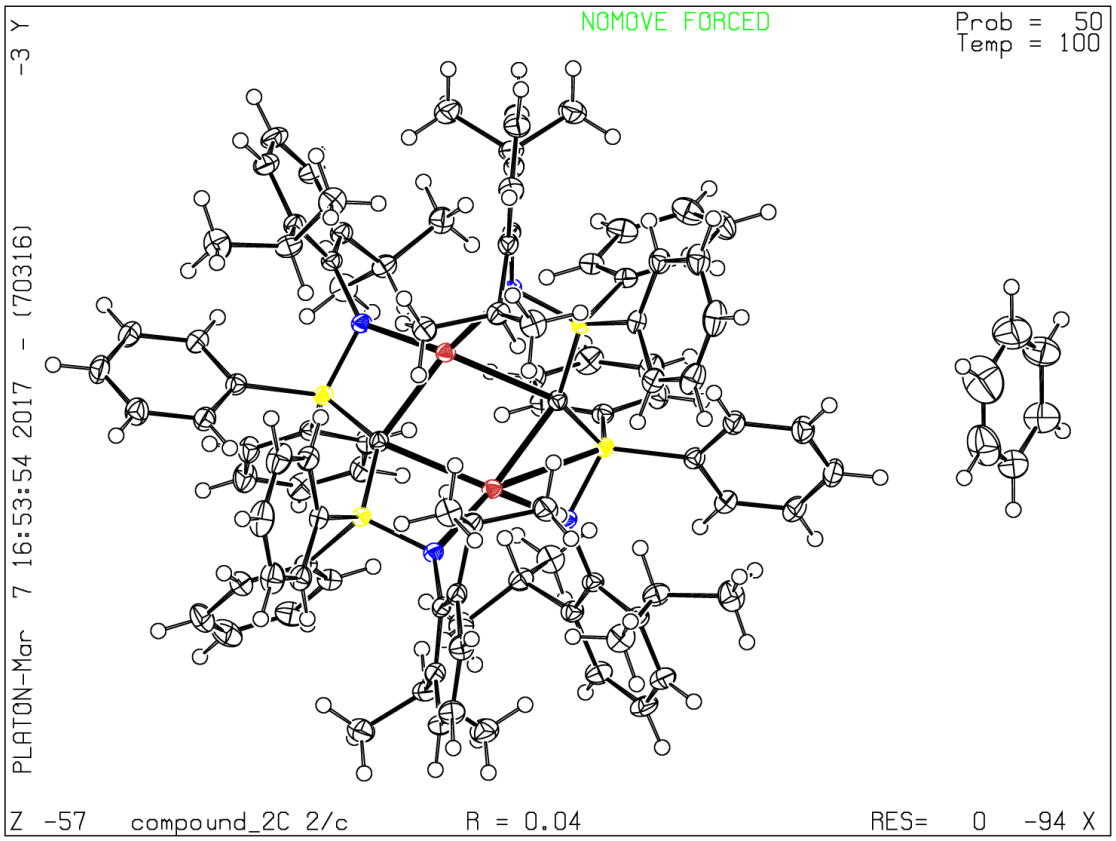
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 26/02/2017; check.def file version of 21/02/2017

Datablock compound_2'' - ellipsoid plot



checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_2’’’

```
Bond precision:  C-C = 0.0057 A          Wavelength=0.71080

Cell:          a=13.510(3)       b=14.400(3)      c=29.430(6)
               alpha=100.84(3)   beta=100.81(3)   gamma=100.62(3)
Temperature:   100 K
```

	Calculated	Reported
Volume	5379(2)	5379(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C98 H108 Mg2 N4 P4 [+ solvent]	?
Sum formula	C98 H108 Mg2 N4 P4 [+ solvent]	C114 H140 Mg2 N4 O4 P4
Mr	1514.39	1802.79
Dx,g cm-3	0.935	1.113
Z	2	2
Mu (mm-1)	0.119	0.133
F000	1616.0	1936.0
F000’	1617.41	
h,k,lmax	17,18,37	17,18,37
Nref	23807	23560
Tmin,Tmax	0.994,0.996	0.992,0.995
Tmin’	0.993	

```
Correction method= # Reported T Limits: Tmin=0.992 Tmax=0.995
AbsCorr = MULTI-SCAN

Data completeness= 0.990          Theta(max)= 27.131

R(reflections)= 0.0779( 14069)    wR2(reflections)= 0.2280( 23560)

S = 1.001                 Npar= 989
```

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 1802.79
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	98.00	1177.08
H	1.01	108.00	108.86
N	14.01	4.00	56.03
O	16.00	0.00	0.00
Mg	24.31	2.00	48.61
P	30.97	4.00	123.90

Calculated formula weight 1514.48

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C87 -- C92 .. 7.5 s.u.
PLAT990_ALERT_1_B Deprecated RES file style based SQUEEZE job .... ! Note

---

Alert level C

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00572 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H4 .. H28 . 1.90 Ang.

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C114 H140 Mg2 N4 O4 P4
Atom count from the _atom_site data: C98 H108 Mg2 N4 P4
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C114 H140 Mg2 N4 O4 P4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	228.00	196.00	32.00
H	280.00	216.00	64.00
Mg	4.00	4.00	0.00
N	8.00	8.00	0.00
O	8.00	0.00	8.00
P	8.00	8.00	0.00

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum found in CIF ..... Please Check
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum found in CIF ..... Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.03 Degree
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note

```
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C1 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C2 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
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 ...         17 Note
PLAT984_ALERT_1_G The Mg-f'=     0.049 Deviates from the B&C-Value      0.050 Check
```

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

 11 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
  1 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

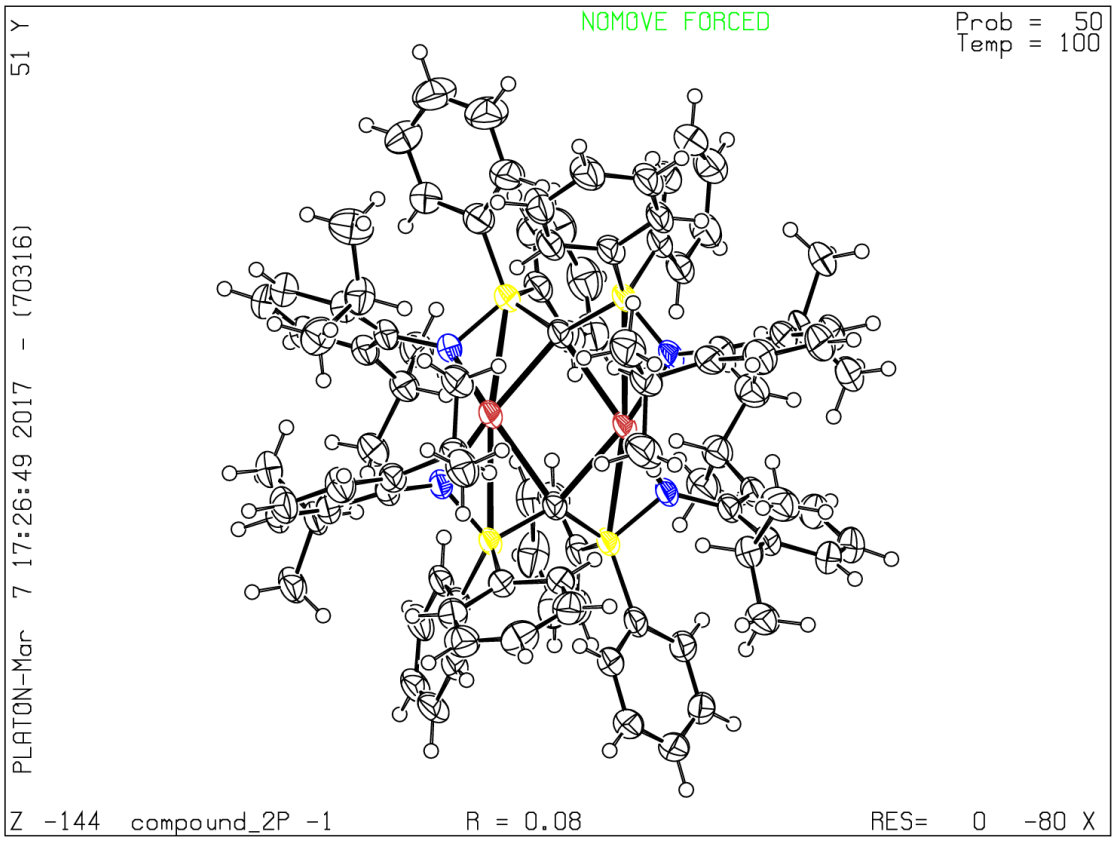
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 26/02/2017; check.def file version of 21/02/2017

Datablock compound_2''' - ellipsoid plot



checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_3

```
Bond precision:  C-C = 0.0019 A          Wavelength=0.71073

Cell:            a=13.149(3)     b=18.972(4)        c=17.427(4)
                 alpha=90        beta=99.58(3)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	4286.8(17)	4286.8(15)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C49 H57 Al N2 P2	?
Sum formula	C49 H57 Al N2 P2	C49 H57 Al N2 P2
Mr	762.89	762.88
Dx,g cm-3	1.182	1.182
Z	4	4
Mu (mm-1)	0.155	0.157
F000	1632.0	1632.0
F000’	1633.50	
h,k,lmax	17,25,23	17,25,22
Nref	10982	10752
Tmin,Tmax	0.992,0.995	0.991,0.996
Tmin’	0.992	

```
Correction method= # Reported T Limits: Tmin=0.991 Tmax=0.996
AbsCorr = MULTI-SCAN

Data completeness= 0.979          Theta(max)= 28.604

R(reflections)= 0.0384( 10060)    wR2(reflections)= 0.1021( 10752)

S = 1.048                 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 G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum found in CIF ........     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          2 Units
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 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

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

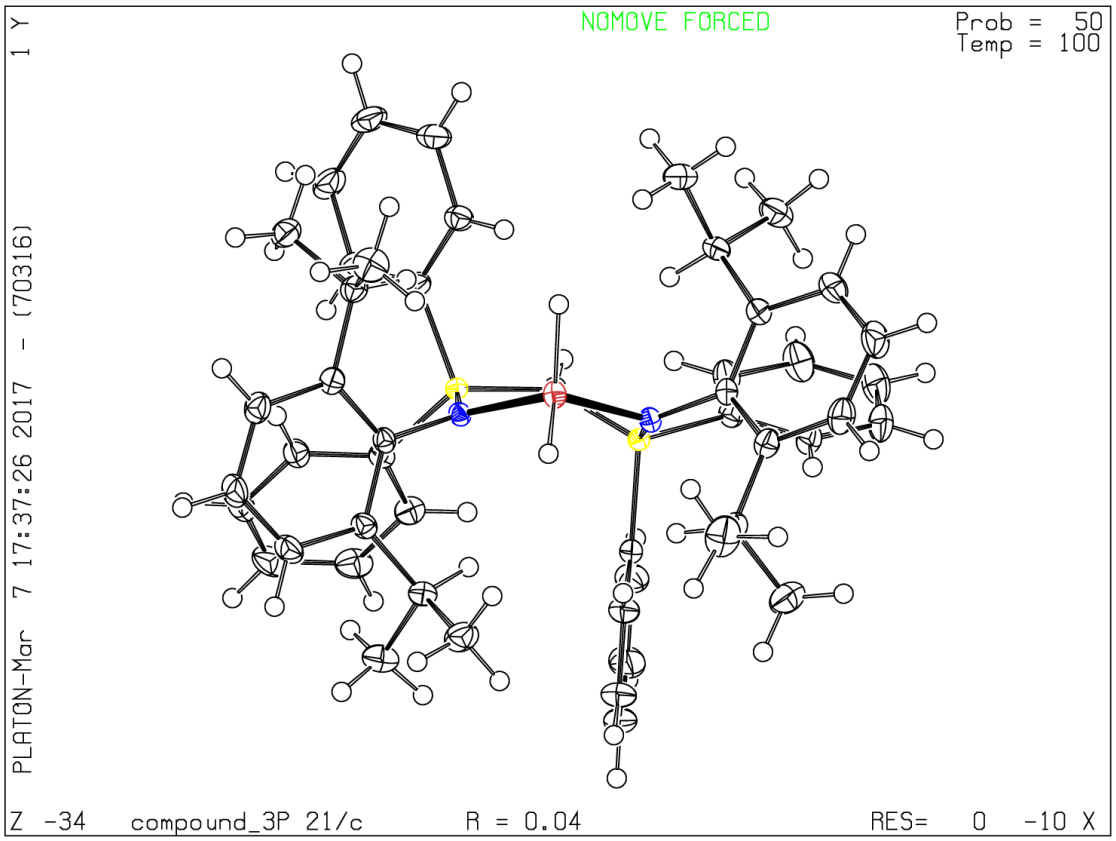
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 26/02/2017; check.def file version of 21/02/2017

Datablock compound_3 - ellipsoid plot