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: NZ1390

```
Bond precision:  C-C = 0.0130 A          Wavelength=0.71073

Cell:            a=27.611(2)     b=18.2397(7)     c=28.2449(10)
                 alpha=90        beta=90          gamma=90
Temperature:     150 K
```

	Calculated	Reported
Volume	14224.6(13)	14224.5(13)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C75 H66 Ag3 Cl2 P6, F6 P	?
Sum formula	C75 H66 Ag3 Cl2 F6 P7	C75 H66 Ag3 Cl2 F6 P7
Mr	1692.58	1692.57
Dx,g cm-3	1.581	1.581
Z	8	8
Mu (mm-1)	1.109	1.109
F000	6800.0	6800.0
F000’	6788.88	
h,k,lmax	37,25,38	35,24,38
Nref	19371	17065
Tmin,Tmax	0.899,0.957	0.777,1.000
Tmin’	0.810	

```
Correction method= # Reported T Limits: Tmin=0.777 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.881          Theta(max)= 29.262

R(reflections)= 0.0817( 7437)     wR2(reflections)= 0.1725( 17065)

S = 0.996                 Npar= 839
```

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 C59 has ADP max/min Ratio ..... 5.7 prolat

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

PLAT222_ALERT_3_A Large Non-Solvent H Uiso(max)/Uiso(min) ... 10.0 Ratio

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

PLAT241_ALERT_2_A High Ueq as Compared to Neighbors for ..... C58 Check

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

Alert level B

PLAT213_ALERT_2_B Atom C58 has ADP max/min Ratio ..... 5.0 prolat

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C54 Check
PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C57 Check
PLAT331_ALERT_2_B Small Average Phenyl C-C Dist. C54 -C59 1.36 Ang.
PLAT331_ALERT_2_B Small Average Phenyl C-C Dist. C63 -C68 1.35 Ang.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

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           Rint given   0.172
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........      0.172 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         44 %
PLAT213_ALERT_2_C Atom C57            has ADP max/min Ratio .....        3.3 prolat
```

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

```
PLAT213_ALERT_2_C Atom C68            has ADP max/min Ratio .....        3.3 prolat
```

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference C11    --  C12     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C67    --  C68     ..       0.20 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C11 Check
```

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

```
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C59 Check
```

Author Response: There is some disorder/large thermal parameters associated with a single phenyl ring of a dppm molecule (C54-C59 and associated hydrogen atoms). The phenyl ring in question is directed into a cavity formed by the dppm ligands of an adjacent complex. Attempts to model this disorder were unsuccesful.

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C56 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0130 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        31 Ang3
```

Alert level G

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  Cl4     ..        7.9 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  Cl4     ..        7.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag3    --  Cl5     ..        7.0 su
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of        P90 Check
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          2 Units
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   3 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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  5 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 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
  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*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock NZ1390 - ellipsoid plot