checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: aa704

```
Bond precision:  C-C = 0.0138 A          Wavelength=0.71069

Cell:          a=10.657(1)        b=15.472(1)      c=19.027(1)
               alpha=101.860(1)   beta=94.240(1)   gamma=104.373(1)
Temperature:   150 K
```

	Calculated	Reported
Volume	2948.3(4)	2948.2(4)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C60 H78 N3 O3 P2 Y	C60 H78 N3 O3 P2 Y, 1/2 (C5 H12)
Sum formula	C60 H78 N3 O3 P2 Y	C62.50 H84 N3 O3 P2 Y
Mr	1040.11	1076.18
Dx,g cm-3	1.172	1.212
Z	2	2
Mu (mm-1)	1.086	1.089
F000	1104.0	1146.0
F000’	1099.15	
h,k,lmax	11,16,20	11,16,20
Nref	7197	6749
Tmin,Tmax	0.925,0.957	0.863,0.958
Tmin’	0.859	

```
Correction method= MULTI-SCAN

Data completeness= 0.938          Theta(max)= 21.970

R(reflections)= 0.0839( 4740)     wR2(reflections)= 0.1817( 6749)

S = 1.102                 Npar= 641
```

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

```
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.5264
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.938
```

PLAT073_ALERT_1_A H-atoms ref, but _hydrogen_treatment reported as constr

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Alert level B

PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 183 A**3

Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 1076.18
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	60.00	720.66
H	1.01	78.00	78.62
N	14.01	3.00	42.02
O	16.00	3.00	48.00
P	30.97	2.00	61.95
Y	88.91	1.00	88.91

Calculated formula weight 1040.16

REFLT03_ALERT_3_C Reflection count < 95% complete
From the CIF: _diffrn_reflns_theta_max 21.97
From the CIF: _diffrn_reflns_theta_full 21.97
From the CIF: _reflns_number_total 6749
TEST2: Reflns within _diffrn_reflns_theta_max
Count of symmetry unique reflns 7197
Completeness (_total/calc) 93.78%

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT043_ALERT_1_C Check Reported Molecular Weight 1076.18
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 6.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C15 -- C17 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C46 -- C47 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C47 -- C48 .. 0.17 Ang.
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C41
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C57
PLAT245_ALERT_2_C U(iso) H2N Smaller than U(eq) N2 by ... 0.014 AngSq
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0138 Ang
PLAT420_ALERT_2_C D-H Without Acceptor N2 - H2N ... ?

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:C62.5 H84 N3 O3 P2 Y1
Atom count from the _atom_site data: C60 H78 N3 O3 P2 Y1

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 C62.50 H84 N3 O3 P2 Y
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	125.00	120.00	5.00
H	168.00	156.00	12.00
N	6.00	6.00	0.00
O	6.00	6.00	0.00
P	4.00	4.00	0.00

```
          Y          2.00      2.00    0.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      15.06
PLAT153_ALERT_1_G The su's on the Cell Axes   are Equal .........    0.00100 Ang.
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........    0.00100 Deg.
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   3 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   8 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
   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
```

Datablock: pa679bis

Bond precision: C-C = 0.0063 A Wavelength=0.71069

Cell: a=27.529(1) b=28.356(1) c=18.325(1)
       alpha=90 beta=124.463(1) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	11794.1(9)	11794.1(9)
Space group	C 2/c	C2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C114 H144 N6 O6 P4 Y2	C114 H144 N6 O6 P4 Y2, 2(C6 H12)
Sum formula	C114 H144 N6 O6 P4 Y2	C126 H168 N6 O6 P4 Y2
Mr	1996.05	2164.36
Dx,g cm-3	1.124	1.219
Z	4	4
Mu (mm-1)	1.084	1.089
F000	4224.0	4608.0
F000'	4204.54	
h,k,lmax	33,34,22	33,34,22
Nref	11614	11468
Tmin,Tmax	0.787,0.804	0.796,0.812
Tmin'	0.787	

Correction method= MULTI-SCAN

Data completeness= 0.987 Theta(max)= 26.020

R(reflections)= 0.0565(8593) wR2(reflections)= 0.1259(11468)

S = 1.050 Npar= 635

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

PLAT073_ALERT_1_A H-atoms ref, but _hydrogen_treatment reported as constr

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Alert level B

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.95 <> 1.05
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 2164.36
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	114.00	1369.25
H	1.01	144.00	145.15
N	14.01	6.00	84.04
O	16.00	6.00	95.99
P	30.97	4.00	123.90
Y	88.91	2.00	177.81

Calculated formula weight 1996.15

PLAT420_ALERT_2_B D-H Without Acceptor O4 - H4O ... ?

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C15 -- C16B .. 6.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for C15 -- C18B .. 6.0 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C23
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C41
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0063 Ang
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF: Y1 -- Y1 .. 3.92 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:C126 H168 N6 O6 P4 Y2
Atom count from the _atom_site data: C114 H144 N6 O6 P4 Y2
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 C126 H168 N6 O6 P4 Y2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	504.00	456.00	48.00
H	672.00	576.00	96.00
N	24.00	24.00	0.00
O	24.00	24.00	0.00
P	16.00	16.00	0.00

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           Y          8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      50.84
PLAT153_ALERT_1_G The su's on the Cell Axes   are Equal .........    0.00100 Ang.
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          6 Perc.
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .        459 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         43
              C57  -O3   -C57     2.655   1.555   1.555             23.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        134
              C16A -C15  -C16B    1.555   1.555   1.555             31.80 Deg.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          9
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
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   4 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

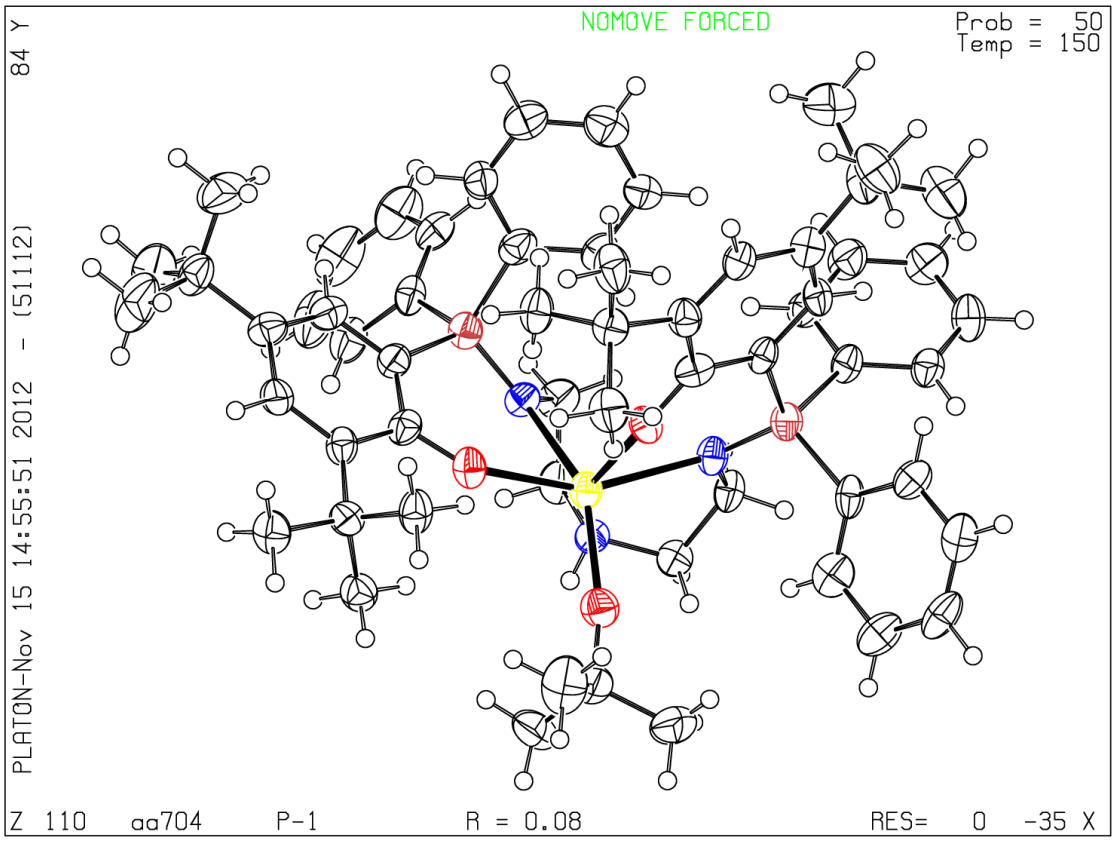
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 05/11/2012; check.def file version of 05/11/2012

Datablock aa704 - ellipsoid plot



Datablock pa679bis - ellipsoid plot