checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kckg1

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kckg1

```
Bond precision:  C-C = 0.0174 A          Wavelength=0.71073

Cell:           a=13.4400(19)    b=17.383(2)         c=13.2418(17)
                alpha=90         beta=104.546(13)    gamma=90
Temperature:    293 K
```

	Calculated	Reported
Volume	2994.5(7)	2994.5(7)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C28 H42 N4 O P2	?
Sum formula	C28 H42 N4 O P2	C28 H42 N4 O P2
Mr	512.60	512.60
Dx,g cm-3	1.137	1.137
Z	4	4
Mu (mm-1)	0.171	0.171
F000	1104.0	1104.0
F000’	1105.14	
h,k,lmax	15,20,15	15,20,15
Nref	5261	4580
Tmin,Tmax	0.968,0.983	0.957,1.000
Tmin’	0.966	

```
Correction method= EMPIRICAL

Data completeness= 0.871          Theta(max)= 25.000

R(reflections)= 0.1372( 1974)     wR2(reflections)= 0.3537( 4580)

S = 1.011                 Npar= 332
```

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.871

Alert level B

```
REFLT03_ALERT_3_B  Reflection count < 90% complete (theta max?)
           From the CIF: _diffrn_reflns_theta_max          25.00
           From the CIF: _diffrn_reflns_theta_full         25.00
           From the CIF: _reflns_number_total              4580
           TEST2: Reflns within _diffrn_reflns_theta_max
           Count of symmetry unique reflns         5261
           Completeness (_total/calc)             87.06%
RFACR01_ALERT_3_B  The value of the weighted R factor is > 0.35
            Weighted R factor given   0.354
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        4.6 Ratio
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.0174 Ang
```

Alert level C

```
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
            R factor given   0.137
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         43 Perc.
PLAT082_ALERT_2_C High R1 Value ..................................       0.14
PLAT084_ALERT_2_C High wR2 Value .................................       0.35
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.37
PLAT213_ALERT_2_C Atom C4              has ADP max/min Ratio .....        3.1 prola
PLAT234_ALERT_4_C Large Hirshfeld Difference C9     --  C11     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22    --  C23     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23    --  C24     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C24    --  C25     ..       0.19 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C5
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C9
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C22
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3D    ...          ?
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         41 A**3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.12
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       8.42
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          1
```

```
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   4 ALERT level B = A potentially serious problem, consider carefully
  16 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

   3 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
   7 ALERT type 3 Indicator that the structure quality may be low
   5 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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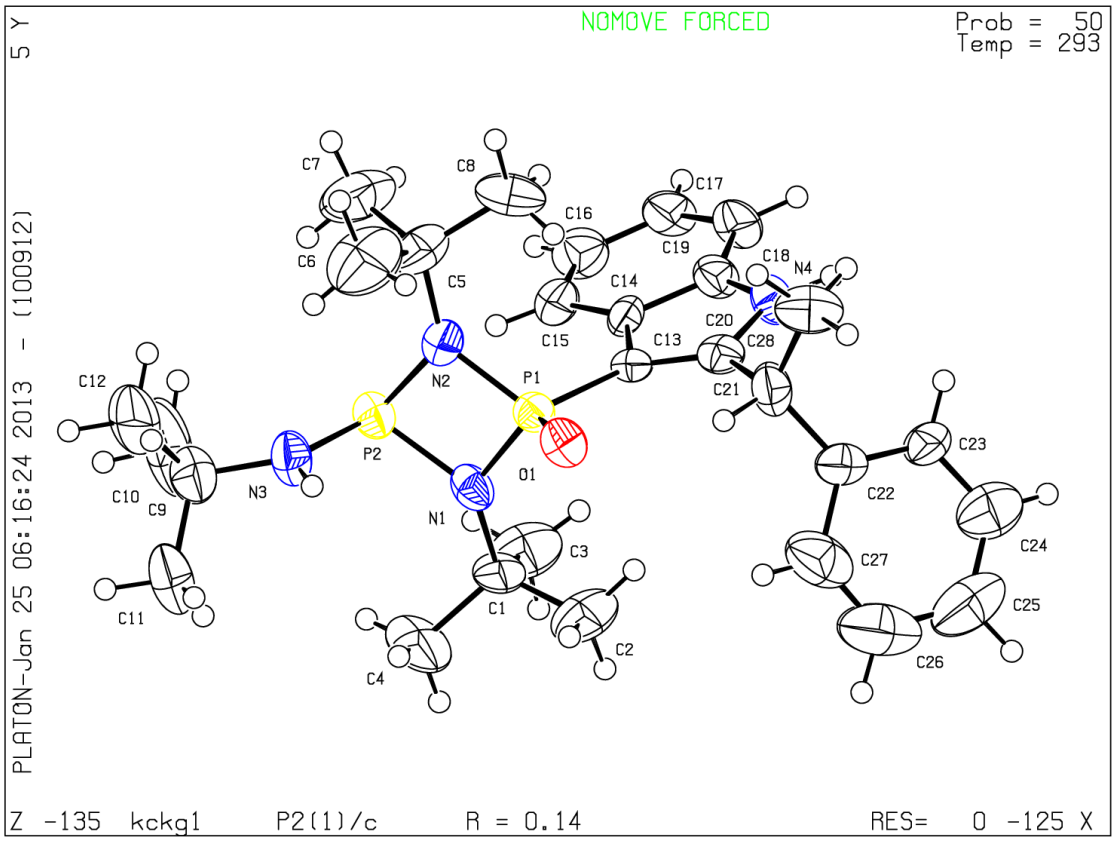
PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock kckg1 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kck517a_m

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kck517a_m

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:            a=21.035(4)     b=10.233(2)         c=15.523(3)
                 alpha=90        beta=128.87(3)      gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	2601.5(14)	2601.4(9)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C24 H26 N4 O6 P2	?
Sum formula	C24 H26 N4 O6 P2	C24 H26 N4 O6 P2
Mr	528.43	528.43
Dx,g cm-3	1.349	1.349
Z	4	4
Mu (mm-1)	0.213	0.213
F000	1104.0	1104.0
F000’	1105.30	
h,k,lmax	24,12,18	24,12,18
Nref	2290	2294
Tmin,Tmax	0.946,0.962	0.946,0.962
Tmin’	0.946	

```
Correction method= EMPIRICAL

Data completeness= 1.002          Theta(max)= 24.990

R(reflections)= 0.0411( 1911)     wR2(reflections)= 0.1149( 2294)

S = 1.037                 Npar= 166
```

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

CELLV02_ALERT_1_B The supplied cell volume s.u. differs from that calculated from the cell parameter s.u.’s by > 4
Calculated cell volume su = 14.01
Cell volume su given = 9.00

Alert level C

```
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C1
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.1. Differ by ...          5 Units
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          8
              N1   -P1   -P1      2.555   1.555   2.555             42.94 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #          9
              N1   -P1   -P1      1.555   1.555   2.555             42.36 Deg.
```

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

   7 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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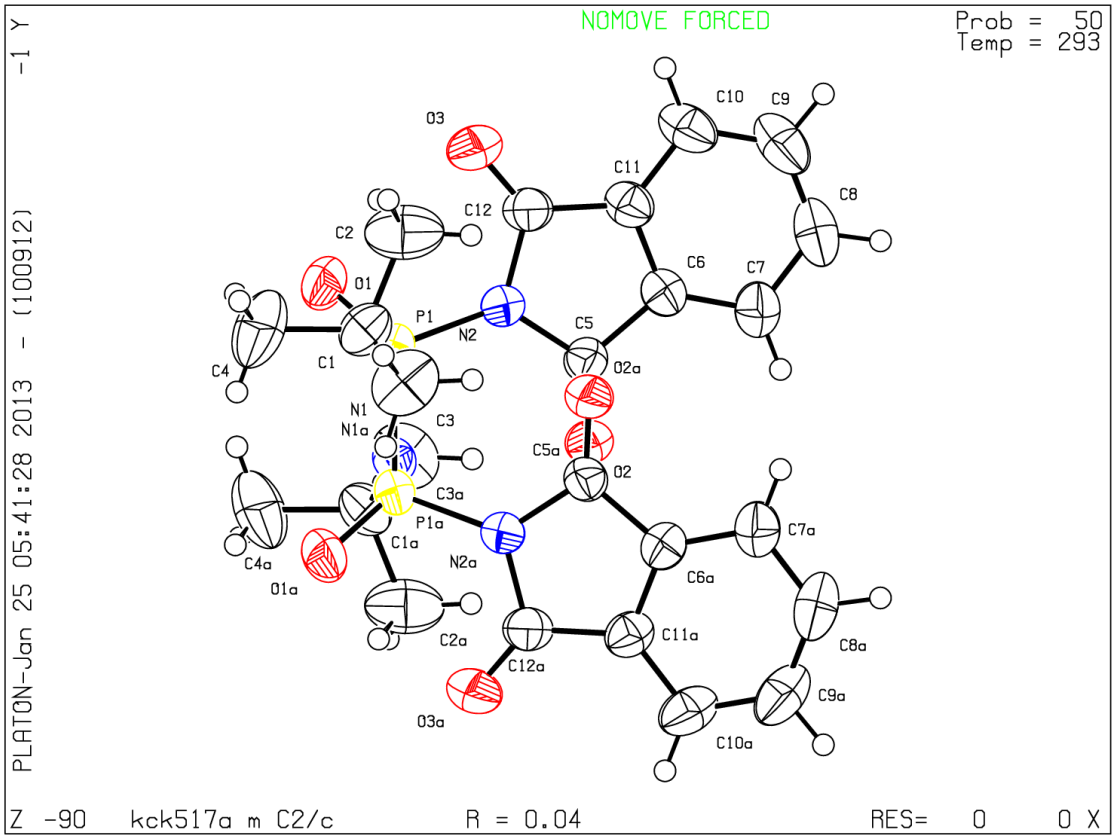
PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock kck517a_m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) platon

No syntax errors found. CIF dictionary Interpreting this report

Datablock: platon

```
Bond precision:  C-C = 0.0144 A          Wavelength=0.71073

Cell:         a=7.9645(14)      b=9.0060(12)     c=22.375(3)
              alpha=95.477(11)  beta=93.033(13)  gamma=113.752(15)
Temperature:  293 K
```

	Calculated	Reported
Volume	1454.9(4)	1454.9(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C24 H26 N4 O6 P2, C H2 Cl2	?
Sum formula	C25 H28 Cl2 N4 O6 P2	C25 H28 Cl2 N4 O6 P2
Mr	613.35	613.35
Dx,g cm-3	1.400	1.400
Z	2	2
Mu (mm-1)	0.379	0.379
F000	636.0	636.0
F000’	637.25	
h,k,lmax	9,10,26	9,10,26
Nref	5133	5019
Tmin,Tmax	0.920,0.934	0.920,1.000
Tmin’	0.920	

```
Correction method= EMPIRICAL

Data completeness= 0.978          Theta(max)= 25.000

R(reflections)= 0.1331( 3485)     wR2(reflections)= 0.3184( 5019)

S = 1.067                 Npar= 359
```

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0144 Ang

---

Alert level C

```
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
           R factor given   0.133
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.318
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.978
PLAT082_ALERT_2_C High R1 Value ..................................      0.13
PLAT084_ALERT_2_C High wR2 Value .................................      0.32
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C13
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C25
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF         ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     13.78
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .     mixed
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         8
             N1   -P1   -P1      1.555   1.555   2.656            42.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         9
             N1   -P1   -P1      2.656   1.555   2.656            41.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        72
             N3   -P2   -P2      2.555   1.555   2.555            43.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        73
             N3   -P2   -P2      1.555   1.555   2.555            42.90 Deg.
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   4 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
   4 ALERT type 3 Indicator that the structure quality may be low
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   1 ALERT type 5 Informative message, check
```

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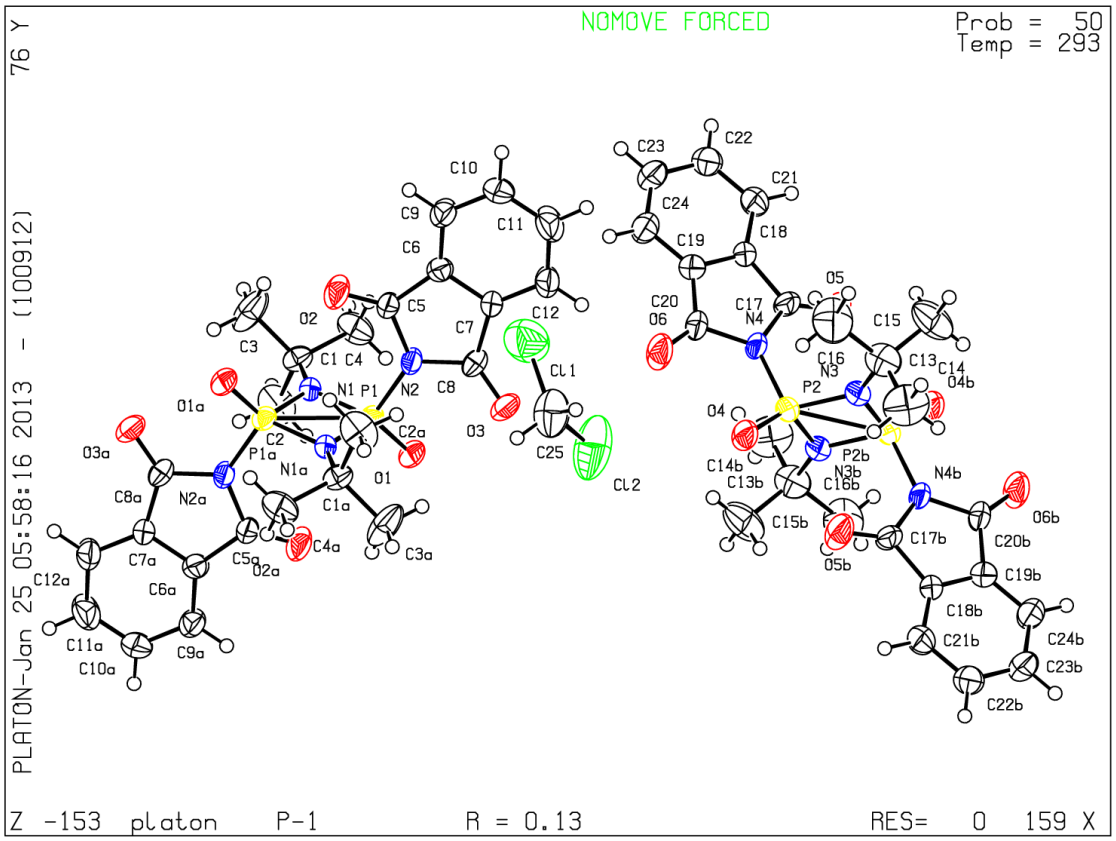
PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock platon - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kck496a

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kck496a

```
Bond precision:  C-C = 0.0061 A          Wavelength=0.71073

Cell:             a=18.116(4)     b=10.276(2)        c=11.554(2)
                  alpha=90        beta=90.29(3)      gamma=90
Temperature:      293 K
```

	Calculated	Reported
Volume	2150.9(7)	2150.7(7)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C16 H32 N4 O3 P2	?
Sum formula	C16 H32 N4 O3 P2	C16 H32 N4 O3 P2
Mr	390.40	390.40
Dx,g cm-3	1.206	1.206
Z	4	4
Mu (mm-1)	0.223	0.223
F000	840.0	840.0
F000’	841.10	
h,k,lmax	21,12,13	21,12,13
Nref	3785	3629
Tmin,Tmax	0.948,0.956	0.948,0.956
Tmin’	0.948	

```
Correction method= EMPIRICAL

Data completeness= 0.959          Theta(max)= 25.000

R(reflections)= 0.0740( 2766)     wR2(reflections)= 0.1609( 3629)

S = 1.094                 Npar= 262
```

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

```
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low .......      0.959
PLAT215_ALERT_3_B Disordered C12B      has ADP max/min Ratio .....        4.4
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        6.2 Ratio
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for         C9
```

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.43
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        6.7 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C5
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0061 Ang
PLAT751_ALERT_4_C Bond    Calc     0.00000, Rep   0.000(10) ......  Senseless su
              O2   -O2      1.555   1.555                   #         14
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................         12 Perc.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         22
              O2   -O2   -C13     1.555   1.555   1.555              0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         23
              O2   -C13  -O2      1.555   1.555   1.555              0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         58
              C10A -C9   -C10B    1.555   1.555   1.555             44.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         62
              C11A -C9   -C11B    1.555   1.555   1.555             41.30 Deg.
```

```
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```

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PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock kck496a - ellipsoid plot