

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: dl179d

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Bond precision:    C-C = 0.0080 A                      Wavelength=0.71073

Cell:              a=14.6617(14)            b=12.9745(12)            c=20.0336(19)  
                    alpha=90                      beta=90                      gamma=90

Temperature:      180 K

	Calculated	Reported
Volume	3811.0(6)	3811.0(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C14 H32 N2 P, I	C14 H32 N2 P, I
Sum formula	C14 H32 I N2 P	C14 H32 I N2 P
Mr	386.29	386.29
Dx,g cm-3	1.347	1.347
Z	8	8
Mu (mm-1)	1.755	1.755
F000	1584.0	1584.0
F000'	1581.38	
h,k,lmax	18,16,24	18,15,24
Nref	3767	3722
Tmin,Tmax	0.663,0.810	0.721,0.807
Tmin'	0.585	

Correction method= REFDELTA

Data completeness= 0.988                      Theta(max)= 26.070

R(reflections)= 0.0473( 2480)              wR2(reflections)= 0.1376( 3722)

S = 1.006                                      Npar= 172

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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.

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### Alert level C

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density ....              3.39

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- 0 ALERT level A = In general: serious problem
- 0 ALERT level B = Potentially serious problem
- 1 ALERT level C = Check and explain

0 ALERT level G = General alerts; check  
0 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

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### **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.**

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**PLATON version of 13/08/2009; check.def file version of 12/08/2009**

