

checkCIF/PLATON report

No syntax errors found.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: tha

Bond precision:	C-C = 0.0017 A	Wavelength=0.71073
Cell:	a=7.0320(19)	b=14.376(4)
	alpha=90	beta=93.737(5)
		gamma=90
	Calculated	Reported
Volume	1630.7(8)	1630.7(8)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C6 H9 Be N2 O6, C6 H5 N2 O4, H2 O	?
Sum formula	C12 H16 Be N4 O11	C12 H16 Be N4 O11
Mr	401.30	401.30
Dx,g cm-3	1.635	1.635
Z	4	4
Mu (mm-1)	0.144	0.144
F000	832.0	832.0
F000'	832.57	
h,k,lmax	8,18,20	8,17,20
Nref	3355	3318
Tmin,Tmax	0.939,0.960	
Tmin'	0.939	
Correction method= Not given		
Data completeness= Ratio = 0.99	Theta(max)= 26.45	
R(reflections)= 0.0289(2839)	wR2(reflections)= 0.0796(3318)	
S = 1.041	Npar= 319	

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 C

PLAT432_ALERT_2_C	Short Inter X...Y Contact O8 .. C5 ..	2.97 Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact C4 .. C4 ..	3.15 Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1
	C6 H9 Be N2 O6	
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	2
	C6 H5 N2 O4	
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	3
	H2 O	

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- 0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
5 **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
2 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
3 ALERT type 4 Improvement, methodology, query or suggestion
-

Publication of your CIF in IUCr journals

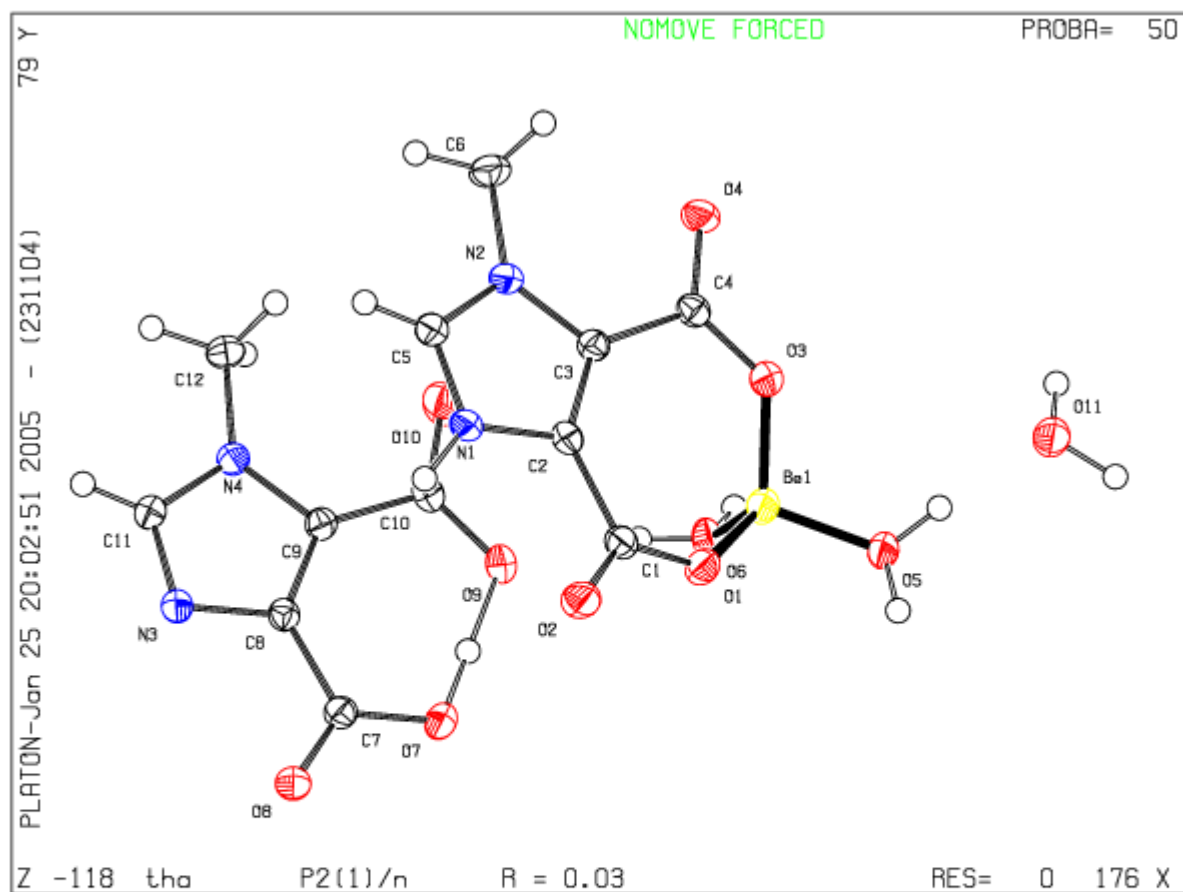
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 23/11/2004; check.def file version of 17/11/2004

Datablock tha - ellipsoid plot



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