

checkCIF/PLATON report (full structural check)

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: PHIE

Bond precision:	C-C = 0.0067 Å	Wavelength=0.71073
Cell:	a=8.3118(4) b=11.0919(4) c=27.7131(15)	
	alpha=90 beta=90 gamma=90	
	Calculated	Reported
Volume	2555.0(2)	2555.0(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C28 H29 N2 O P S	C28 H29 N2 O P S
Sum formula	C28 H29 N2 O P S	C28 H29 N2 O P S
Mr	472.57	472.60
Dx, g cm-3	1.229	1.229
Z	4	4
Mu (mm-1)	0.212	0.212
F000	1000.0	1000.0
F000'	1001.22	
h,k,lmax	10,13,34	10,13,34
Nref	2873(5022)	5000
Tmin,Tmax	0.970,0.987	0.941,0.987
Tmin'	0.903	
Correction method=	AbsCorr=NUMERICAL	
Data completeness=	1.74(1.00) Theta(max)= 26.000	
R(reflections)=	0.0360(3544) wR2(reflections)= wR= 0.0390(5000)	
S =	1.640 Npar= 299	

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

[PLAT761_ALERT_1_A](#) CIF Contains no X-H Bonds ?
[PLAT762_ALERT_1_A](#) CIF Contains no X-Y-H or H-Y-H Angles ?

Alert level C

[PLAT152_ALERT_1_C](#) Supplied and Calc Volume s.u. Inconsistent ?
[PLAT245_ALERT_2_C](#) U(iso) H5 Smaller than U(eq) C5 by ... 0.01 AngSq
[PLAT340_ALERT_3_C](#) Low Bond Precision on C-C Bonds (x 1000) Ang ... 7

Alert level G

[REFLT03_ALERT_4_G](#) Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffn_refl_theta_max 26.00
From the CIF: _reflns_number_total 5000
Count of symmetry unique reflns 2873
Completeness (_total/calc) 174.03%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2127
Fraction of Friedel pairs measured 0.740
Are heavy atom types Z>Si present yes
[PLAT791_ALERT_1_G](#) Confirm the Absolute Configuration of C1 = . S
[PLAT791_ALERT_1_G](#) Confirm the Absolute Configuration of C2 = . S
[PLAT791_ALERT_1_G](#) Confirm the Absolute Configuration of C15 = . R

- 2 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
4 **ALERT level G** = General alerts; check

- 6 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
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF

A full structural check has been run on your CIF. This includes checks on:

- CIF syntax and construction
- Cell and geometry details
- Space-group symmetry
- Anisotropic displacement parameters

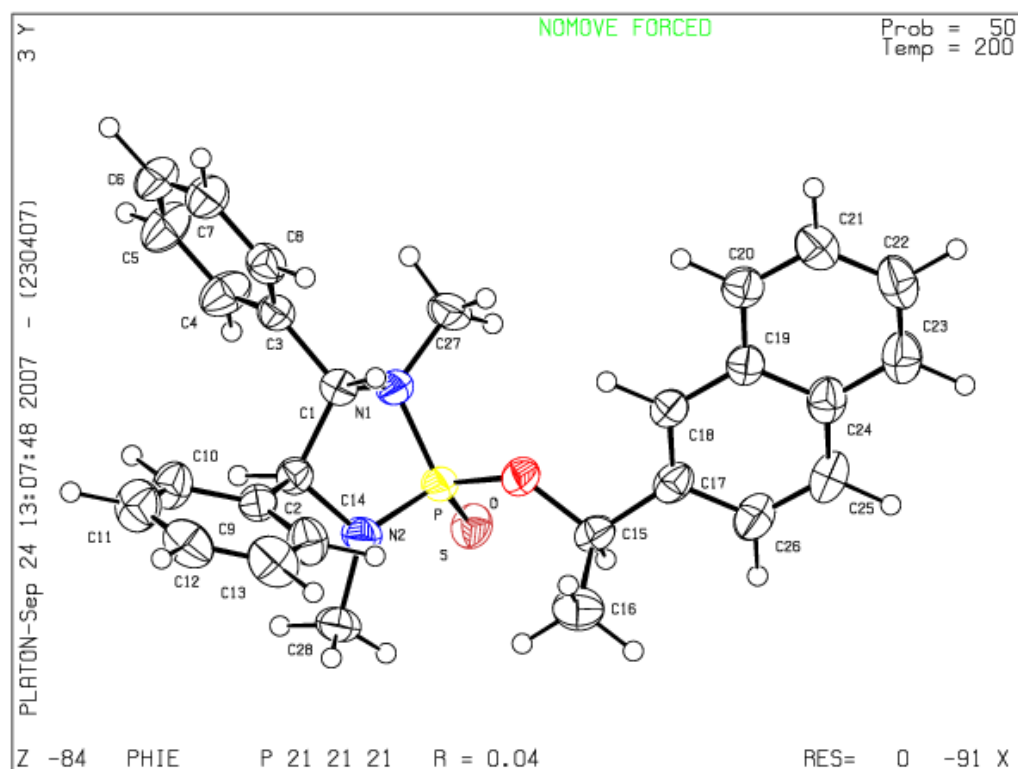
These full checks give an indication of potential problems with your CIF. Please note that if you intend to submit your CIF for publication in Acta Crystallographica Section C or E, you must make sure that [full publication checks](#) are run on the final version of the CIF prior to submission.

If you intend to submit to another section of Acta Crystallographica, Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least [basic structural checks](#) are run on the final version of your CIF prior to submission.

To submit your CIF for publication in an IUCr journal click [here](#).

PLATON version of 23/04/2007; check.def file version of 23/04/2007

Datablock PHIE - ellipsoid plot



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