

No syntax errors found.
Please wait while processing

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

Datablock: PiSe_3_0m

Bond precision: C-C = 0.0014 Å Wavelength=0.71073
Cell: a=11.0151(3) b=12.9054(3) c=13.0023(3)
alpha=90 beta=100.0760(6) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1819.83(8)	1819.82(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H20 N2	C25 H20 N2
Sum formula	C25 H20 N2	C25 H20 N2
Mr	348.43	348.43
Dx, g cm ⁻³	1.272	1.272
Z	4	4
Mu (mm ⁻¹)	0.075	0.075
F000	736.0	736.0
F000'	736.25	
h,k,lmax	15,17,17	15,17,17
Nref	5009	5000
Tmin,Tmax	0.957,0.970	
Tmin'	0.957	
Correction method	Not given	
Data completeness	0.998	Theta(max)= 29.392
R(reflections)= 0.0416(4547)		wR2(reflections)= 0.1146(5000)
S = 1.045	Npar= 244	

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

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 8
Report
2 1 0, 1 2 0, 1 0 1, 1 1 1, -1 3 1, 1 2 2,
0 3 2, 1 1 3,

Alert level G

[PLAT480 ALERT 4 G](#) Long H...A H-Bond Reported H20A ..N1 . 2.66 Ang.
[PLAT883 ALERT 1 G](#) No Info/Value for _atom_sites_solution_primary . Please Do !
[PLAT910 ALERT 3 G](#) Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
-1 0 1,
[PLAT913 ALERT 3 G](#) Missing # of Very Strong Reflections in FCF 2 Note
1 2 2, 0 3 2,
[PLAT933 ALERT 2 G](#) Number of HKL-OMIT Records in Embedded .res File 2 Note
-1 0 1, 1 1 1,
[PLAT967 ALERT 5 G](#) Note: Two-Theta Cutoff Value in Embedded .res .. 58.8
Degree
[PLAT969 ALERT 5 G](#) The 'Henn et al.' R-Factor-gap value 6.003 Note
Predicted wR2: Based on SigI**2 1.91 or SHELX Weight 10.97
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 25 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 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
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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* or *IUCrData*, 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 22/08/2024; check.def file version of 21/08/2024

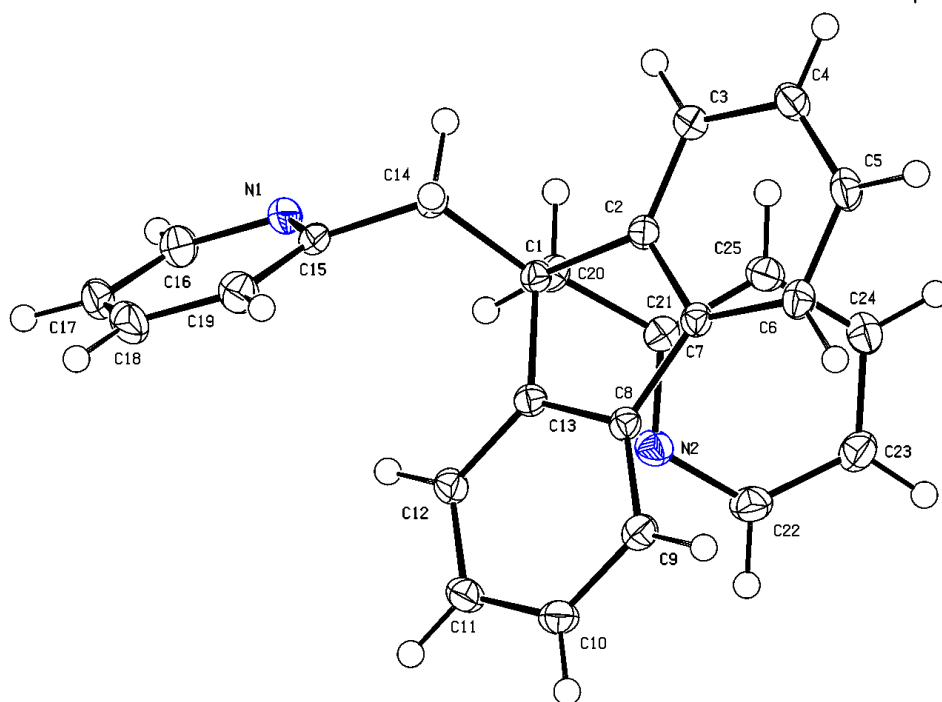
Datablock PiSe_3_0m - ellipsoid plot

31 Y

NOMOVE FORCED

Prob = 50
Temp = 100

PLATON-Oct 21 12:55:25 2024 - (220824)



Z -25

Pl Se_3_0m

P 21/n

R = 0.04

RES= 0 -23 X