checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) panb2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: panb2

Bond precision: C-C = 0.0066 A Wavelength=0.71073

Cell: a=8.8855(4) b=33.1855(18) c=10.2437(5)
alpha=90 beta=97.782(4) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	2992.7(3)	2992.7(3)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P2yn
Moiety formula	C24 H24 Fe2 N O6 P2, B F4, H2 O	C24 H24 Fe2 N O6 P2 +, B F4 -, H2 O
Sum formula	C24 H26 B F4 Fe2 N O7 P2	C24 H26 B F4 Fe2 N O7 P2
Mr	700.91	700.91
Dx,g cm-3	1.556	1.556
Z	4	4
Mu (mm-1)	1.143	1.143
F000	1424.0	1424.0
F000'	1428.31	
h,k,lmax	11,41,12	11,41,12
Nref	6108	6105
Tmin,Tmax	0.792,0.934	0.758,0.937
Tmin'	0.655	

Correction method= # Reported T Limits: Tmin=0.758 Tmax=0.937 AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 26.370

R(reflections)= 0.0465(3147) wR2(reflections)= 0.1070(6105)

S = 0.824 Npar= 383

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

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.150 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1W 0.125 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C19 --C24 . 1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0066 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X H1 ..H7A . 1.97 Ang.
x,y,z = 1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.264 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 1 Report

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C1 . 7.0 s.u.
And 4 other PLAT232 Alerts
More ...
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 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

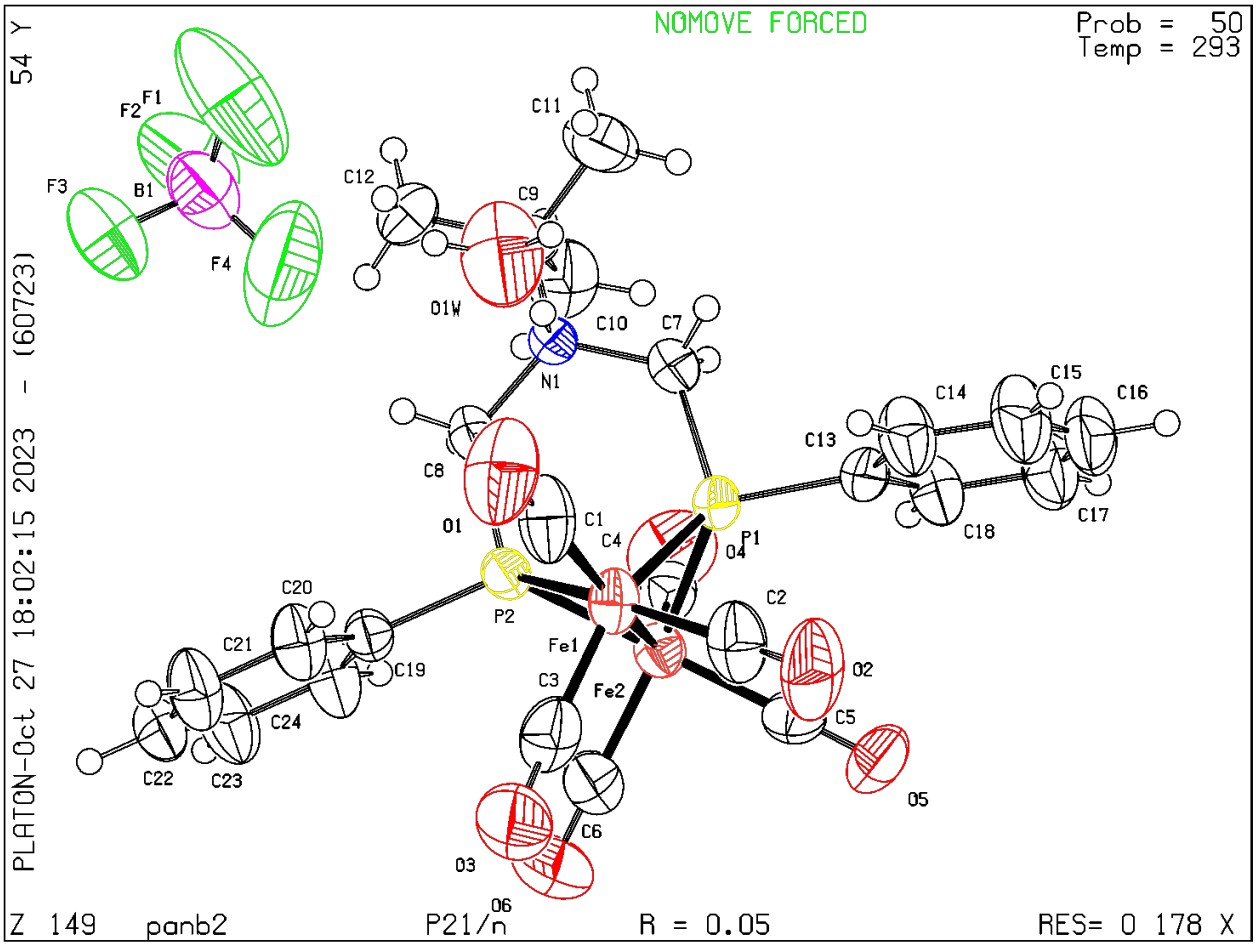
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 06/07/2023; check.def file version of 30/06/2023

Datablock panb2 - ellipsoid plot



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