

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh184_sq

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 Interpreting this report

Datablock: deh184_sq

Bond precision:	C-C = 0.0075 A	Wavelength=0.71073
Cell:	a=22.5089(5)	b=11.2869(3) c=24.3139(6)
	alpha=90	beta=110.718(1) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	5777.6(2)	5777.6(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C50 H40 Ir N8, 3(F6 P), 2(C2 H3 N) [+ solvent]	?
Sum formula	C54 H46 F18 Ir N10 P3 [+ solvent]	C27 H23 F9 Ir0.50 N5 P1.50
Mr	1462.14	731.06
Dx, g cm ⁻³	1.681	1.681
Z	4	8
Mu (mm ⁻¹)	2.499	2.499
F000	2896.0	2896.0
F000'	2893.19	
h,k,lmax	32,16,34	32,16,34
Nref	8910	8885
Tmin,Tmax	0.641,0.681	
Tmin'	0.628	

Correction method= Not given

Data completeness= 0.997 Theta(max)= 30.625

R(reflections)= 0.0380(8688) wR2(reflections)= 0.0947(8885)

S = 1.260 Npar= 387

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

PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for F2	.	2	Check
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C26	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.1	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.9	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	N5	0.106	Check
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H25B ..H27B	.	2.14 Ang.
	-1/2+x,1/2-y,-1/2+z =		8_455	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.133	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		5	Note
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info



Alert level G

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	39.67	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1	--F1	.	5.5 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P1	--F3	.	7.2 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P1	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		P2	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F1	..C24	2.94	Ang.
	1-x,y,1/2-z =		2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F1	..C24	2.94	Ang.
	x,y,z =		1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F5	..C25	2.91	Ang.
	x,y,z =		1_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		24	A**3
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	16	Note

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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 9 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.

