

# checkCIF () running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

## checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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. You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. [CIF dictionary](#)

Please wait while processing .... [Interpreting this report](#)

[Structure factor report](#)

### Datablock: Ir\_2

Bond precision:	C-C = 0.0219 A	Wavelength=0.71073
Cell:	a=9.3075 (8)      b=12.1090 (8)      c=24.6823 (18)	
	alpha=90      beta=90      gamma=90	
Temperature:	295 K	
	Calculated	Reported
Volume	2781.8 (4)	2781.8 (4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C23 H30 Cl Ir N3 O6, F6 P	C23 H30 Cl Ir N3 O6, F6 P
Sum formula	C23 H30 Cl F6 Ir N3 O6 P	C23 H30 Cl F6 Ir N3 O6 P
Mr	817.14	817.12
Dx, g cm-3	1.951	1.951
Z	4	4
Mu (mm-1)	5.038	5.038
F000	1600.0	1600.0
F000'	1596.25	
h, k, lmax	11, 15, 30	11, 15, 30
Nref	5711 [ 3235]	5675
Tmin, Tmax	0.542, 0.678	0.530, 0.700
Tmin'	0.076	
Correction method=	# Reported T Limits: Tmin=0.530 Tmax=0.700	AbsCorr = MULTI-SCAN
Data completeness=	1.75/0.99	Theta (max)= 26.420
R (reflections)=	0.0588 ( 4789)	wR2 (reflections)= 0.1040 ( 5675)
S =	Npar=	
1.070	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 A

[PLAT213 ALERT 2 A](#) Atom C54 has ADP max/min Ratio ..... 6.9 oblate

**Author Response: Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

#### Alert level B

[PLAT213 ALERT 2 B](#) Atom C6' has ADP max/min Ratio ..... 4.1 oblate

**Author Response: Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT342\\_ALERT\\_3\\_B](#) Low Bond Precision on C-C Bonds ..... 0.0219 Ang.

**Author Response: resence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT369\\_ALERT\\_2\\_B](#) Long C(sp2)-C(sp2) Bond C2' - C5 . 1.57 Ang.

**Author Response: resence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT417\\_ALERT\\_2\\_B](#) Short Inter D-H..H-D H4O ..H6O . 1.80 Ang.  
-1/2+x, 3/2-y, 1-z = 2\_466 Check

**Author Response: Orientation of OH is uncertain. resence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT420\\_ALERT\\_2\\_B](#) D-H Bond Without Acceptor O2" --H2O . Please Check

**Author Response: Orientation of OH is uncertain. Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT420\\_ALERT\\_2\\_B](#) D-H Bond Without Acceptor O3" --H3O . Please Check

**Author Response: Orientation of OH is uncertain. Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT420\\_ALERT\\_2\\_B](#) D-H Bond Without Acceptor O6" --H6O . Please Check

**Author Response: Orientation of OH is uncertain. Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT728\\_ALERT\\_1\\_B](#) D-H..A Calc 167.00, Rep 170(20) Dev... 3.00 Degree  
O4" -H4O -O6" 1\_555 1\_555 2\_466 # 3 Check

**Author Response: Orientation of OH is uncertain. Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

#### Alert level C

[PLAT213\\_ALERT\\_2\\_C](#) Atom C2' has ADP max/min Ratio ..... 3.6 prolat

**Author Response: Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C5" has ADP max/min Ratio ..... 3.1 oblate

**Author Response: Presence of very heavy element (Ir) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference O1 --C5 . 0.18 Ang.

#### And 3 other PLAT234 Alerts

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference N1' --C2' . 0.16 Ang.

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference N1' --C6' . 0.19 Ang.

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C2' --C5 . 0.18 Ang.

[PLAT245\\_ALERT\\_2\\_C](#) U(iso) H4O Smaller than U(eq) O4" by 0.017 Ang\*\*2

[PLAT250\\_ALERT\\_2\\_C](#) Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note

[PLAT260\\_ALERT\\_2\\_C](#) Large Average Ueq of Residue Including P1 0.180 Check

[PLAT480\\_ALERT\\_4\\_C](#) Long H...A H-Bond Reported H2O ..F14 . 2.58 Ang.

#### Alert level G

[PLAT002\\_ALERT\\_2\\_G](#) Number of Distance or Angle Restraints on AtSite 8 Note

[PLAT003\\_ALERT\\_2\\_G](#) Number of Uiso or Uij Restrained non-H Atoms ... 5 Report

[PLAT172\\_ALERT\\_4\\_G](#) The CIF-Embedded .res File Contains DFIX Records 1 Report

[PLAT178\\_ALERT\\_4\\_G](#) The CIF-Embedded .res File Contains SIMU Records 1 Report

[PLAT244\\_ALERT\\_4\\_G](#) Low 'Solvent' Ueq as Compared to Neighbors of P1 Check

[PLAT380\\_ALERT\\_4\\_G](#) Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C58 Check

[PLAT395\\_ALERT\\_2\\_G](#) Deviating X-O-Y Angle From 120 for O1 100.6 Degree

[PLAT432\\_ALERT\\_2\\_G](#) Short Inter X...Y Contact Cl1 ..C5 3.21 Ang.

1-x, 1/2+y, 3/2-z = 3\_656 Check

[PLAT720\\_ALERT\\_4\\_G](#) Number of Unusual/Non-Standard Labels ..... 2 Note

[PLAT773\\_ALERT\\_2\\_G](#) Check long C-C Bond in CIF: C3 --C5 2.00 Ang.

[PLAT779\\_ALERT\\_4\\_G](#) Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.50 Deg.

N4 -C3 -C5 1\_555 1\_555 1\_555 ..... # 20 Check

[PLAT779\\_ALERT\\_4\\_G](#) Suspect or Irrelevant (Bond) Angle(s) in CIF ... 44.10 Deg.

N4 -C5 -C3 1\_555 1\_555 1\_555 ..... # 43 Check

[PLAT791\\_ALERT\\_4\\_G](#) Model has Chirality at C1" (Sohnke SpGr) S Verify

#### And 4 other PLAT791 Alerts

[PLAT791\\_ALERT\\_4\\_G](#) Model has Chirality at C2" (Sohnke SpGr) R Verify  
[PLAT791\\_ALERT\\_4\\_G](#) Model has Chirality at C3" (Sohnke SpGr) R Verify  
[PLAT791\\_ALERT\\_4\\_G](#) Model has Chirality at C4" (Sohnke SpGr) S Verify  
[PLAT791\\_ALERT\\_4\\_G](#) Model has Chirality at C5" (Sohnke SpGr) R Verify  
[PLAT860\\_ALERT\\_3\\_G](#) Number of Least-Squares Restraints ..... 34 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 2 ALERT type 3 Indicator that the structure quality may be low  
 17 ALERT type 4 Improvement, methodology, query or suggestion  
 0 ALERT type 5 Informative message, check

### Datablock: Ru\_1

Bond precision: C-C = 0.0306 A Wavelength=0.71073  
 Cell: a=14.531(3) b=24.879(4) c=16.855(4)  
 alpha=90 beta=93.610(5) gamma=90  
 Temperature: 150 K

	Calculated	Reported
Volume	6081(2)	6081(2)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	2(C51 H45 Cl N3 O10 Ru), 2(F6 P), 5(C H Cl3)	2(C51 H45 Cl N3 O10 Ru), 2(F6 P), 5(C H Cl3)
Sum formula	C107 H95 Cl17 F12 N6 O20 P2 Ru2	C107 H95 Cl17 F12 N6 O20 P2 Ru2
Mr	2879.62	2879.61
Dx, g cm <sup>-3</sup>	1.573	1.573
Z	2	2
Mu (mm <sup>-1</sup> )	0.733	0.733
F000	2908.0	2908.0
F000'	2909.76	
h, k, lmax	17, 30, 20	17, 30, 20
Nref	23396[ 11985]	23083
Tmin, Tmax	0.869, 0.965	0.890, 0.970
Tmin'	0.869	

Correction method= # Reported T Limits: Tmin=0.890 Tmax=0.970 AbsCorr = MULTI-SCAN  
 Data completeness= 1.93/0.99 Theta(max)= 25.800  
 R(reflections)= 0.0898( 12753) wR2(reflections)= 0.1753( 23083)  
 S = Npar=  
 1.323 1424

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

[PLAT213\\_ALERT\\_2\\_A](#) Atom C80A has ADP max/min Ratio ..... 5.2 prolat

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT214\\_ALERT\\_2\\_A](#) Atom C93 (Anion/Solvent) ADP max/min Ratio 7.3 prolat

**Author Response: Solvent chloroform is slightly disordered. Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C32A --C33A . 0.37 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

#### Alert level B

[PLAT213\\_ALERT\\_2\\_B](#) Atom C30 has ADP max/min Ratio ..... 4.2 prolat

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_B](#) Atom C75A has ADP max/min Ratio ..... 4.2 prolat

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_B](#) Atom C77A has ADP max/min Ratio ..... 4.4 prolat

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT220\\_ALERT\\_2\\_B](#) NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 6.2 Ratio

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT220\\_ALERT\\_2\\_B](#) NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 6.2 Ratio

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT232\\_ALERT\\_2\\_B](#) Hirshfeld Test Diff (M-X) Ru1 --C74 . 10.5 s.u.

[PLAT232\\_ALERT\\_2\\_B](#) Hirshfeld Test Diff (M-X) Ru2 --C74A . 10.3 s.u.

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C23 --C24 . 0.26 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C24 --C25 . 0.28 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C42 --C43 . 0.26 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C43 --C44 . 0.30 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference C74A --C75A . 0.30 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_B](#) Large Hirshfeld Difference P2 --F23 . 0.28 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT250\\_ALERT\\_2\\_B](#) Large U3/U1 Ratio for Average U(i,j) Tensor .... 4.2 Note

[PLAT260\\_ALERT\\_2\\_B](#) Large Average Ueq of Residue Including Cl61 0.400 Check

**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

[PLAT342\\_ALERT\\_3\\_B](#) Low Bond Precision on C-C Bonds ..... 0.03061 Ang.

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT413\\_ALERT\\_2\\_B](#) Short Inter XH3 .. XHn H32 ..H79D . 1.99 Ang.

1-x, -1/2+y, 1-z = 2\_646 Check

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

#### Alert level C

[PLAT213\\_ALERT\\_2\\_C](#) Atom O30 has ADP max/min Ratio ..... 3.9 prolat

**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C24 has ADP max/min Ratio ..... 3.3 prolat  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C73 has ADP max/min Ratio ..... 3.1 prolat  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C32A has ADP max/min Ratio ..... 3.1 prolat  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C34A has ADP max/min Ratio ..... 3.5 prolat  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT213\\_ALERT\\_2\\_C](#) Atom C45A has ADP max/min Ratio ..... 3.2 prolat  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT214\\_ALERT\\_2\\_C](#) Atom F23 (Anion/Solvent) ADP max/min Ratio 4.5 prolat  
**Author Response: Solvent chloroform is slightly disordered. Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT214\\_ALERT\\_2\\_C](#) Atom C163 (Anion/Solvent) ADP max/min Ratio 4.8 prolat  
**Author Response: Solvent chloroform is slightly disordered. Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT222\\_ALERT\\_3\\_C](#) NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 7.6 Ratio  
[PLAT230\\_ALERT\\_2\\_C](#) Hirshfeld Test Diff for C73 --C74 . 5.8 s.u.  
[PLAT230\\_ALERT\\_2\\_C](#) Hirshfeld Test Diff for C71A --C76A . 5.9 s.u.  
[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference O1" --N2" . 0.18 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C40 --C41 . 0.20 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C45 --C46 . 0.22 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C74 --C75 . 0.17 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference O30A --C30A . 0.22 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C2A' --C3A' . 0.19 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C31A --C36A . 0.24 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference C71A --C72A . 0.25 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference P1 --F11 . 0.16 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT234\\_ALERT\\_4\\_C](#) Large Hirshfeld Difference P1 --F13 . 0.22 Ang.  
**Author Response: Presence of very heavy element (Ru) may caused the problem. Chemical evidence shows that the structure is correct.**

[PLAT241\\_ALERT\\_2\\_C](#) High 'MainMol' Ueq as Compared to Neighbors of C24 Check

#### And 9 other PLAT241 Alerts

<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C43	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C63	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C74	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C33A	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C35A	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C43A	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C45A	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C71A	Check
<a href="#">PLAT241_ALERT_2_C</a>	High	'MainMol'	Ueq as Compared to Neighbors of	C75A	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	Ru1	Check

#### And 10 other PLAT242 Alerts

<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	O3	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C30	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C42	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C78	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	Ru2	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C31A	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C36A	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C76A	Check
<a href="#">PLAT242_ALERT_2_C</a>	Low	'MainMol'	Ueq as Compared to Neighbors of	C78A	Check
<a href="#">PLAT243_ALERT_4_C</a>	High	'Solvent'	Ueq as Compared to Neighbors of	C93	Check
<a href="#">PLAT244_ALERT_4_C</a>	Low	'Solvent'	Ueq as Compared to Neighbors of	C92	Check

#### And 3 other PLAT244 Alerts

<a href="#">PLAT244_ALERT_4_C</a>	Low	'Solvent'	Ueq as Compared to Neighbors of	C94	Check
<a href="#">PLAT244_ALERT_4_C</a>	Low	'Solvent'	Ueq as Compared to Neighbors of	C95	Check
<a href="#">PLAT244_ALERT_4_C</a>	Low	'Solvent'	Ueq as Compared to Neighbors of	C96	Check
<a href="#">PLAT250_ALERT_2_C</a>	Large	U3/U1 Ratio for Average U(i,j) Tensor ...		2.1	Note
<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	P1	0.170	Check

**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	P2	0.169	Check
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**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	C121	0.166	Check
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**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	C131	0.220	Check
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**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	C141	0.209	Check
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**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT260_ALERT_2_C</a>	Large	Average Ueq of Residue Including	C151	0.152	Check
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**Author Response: Solvent chloroform is slightly disordered. Chemical evidence shows that the structure is correct.**

<a href="#">PLAT332_ALERT_2_C</a>	Large	Phenyl C-C Range	C31A	-C36A	.	0.17	Ang.
<a href="#">PLAT336_ALERT_2_C</a>	Long	Bond Distance for .....	C94	-C141	.	1.910	Ang.
<a href="#">PLAT360_ALERT_2_C</a>	Short	C(sp3)-C(sp3) Bond	C78A	- C79A	.	1.35	Ang.
<a href="#">PLAT368_ALERT_2_C</a>	Short	C(sp2)-C(sp2) Bond	C31	- C32	.	1.23	Ang.
<a href="#">PLAT368_ALERT_2_C</a>	Short	C(sp2)-C(sp2) Bond	C34	- C35	.	1.14	Ang.
<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H1A	..F15	.	2.61	Ang.

#### And 5 other PLAT480 Alerts

<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H3	..F21	.	2.58	Ang.
<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H5	..F21	.	2.63	Ang.
<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H5	..F26	.	2.64	Ang.
<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H5A	..F14	.	2.60	Ang.
<a href="#">PLAT480_ALERT_4_C</a>	Long	H...A H-Bond Reported	H5A'	..CL63	.	3.01	Ang.

## Alert level G

<a href="#">PLAT002_ALERT_2_G</a>	Number of Distance or Angle Restraints on AtSite	8	Note
<a href="#">PLAT083_ALERT_2_G</a>	SHELXL Second Parameter in WGHT Unusually Large	11.65	Why ?
<a href="#">PLAT171_ALERT_4_G</a>	The CIF-Embedded .res File Contains EADP Records	1	Report
<a href="#">PLAT172_ALERT_4_G</a>	The CIF-Embedded .res File Contains DFIX Records	1	Report
<a href="#">PLAT175_ALERT_4_G</a>	The CIF-Embedded .res File Contains SAME Records	1	Report
<a href="#">PLAT232_ALERT_2_G</a>	Hirshfeld Test Diff (M-X) Ru2 --C71A	6.0	s.u.
<a href="#">PLAT244_ALERT_4_G</a>	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
<a href="#">PLAT244_ALERT_4_G</a>	Low 'Solvent' Ueq as Compared to Neighbors of	P2	Check
<a href="#">PLAT343_ALERT_2_G</a>	Unusual sp3Angle Range in Main Residue for	C78A	Check
<a href="#">PLAT395_ALERT_2_G</a>	Deviating X-O-Y Angle From 120 for O1"	104.8	Degree
<a href="#">PLAT395_ALERT_2_G</a>	Deviating X-O-Y Angle From 120 for O1A"	106.2	Degree
<a href="#">PLAT432_ALERT_2_G</a>	Short Inter X...Y Contact F16 ..C6'	2.96	Ang.
	x,y,l+z =	1	556 Check
<a href="#">PLAT720_ALERT_4_G</a>	Number of Unusual/Non-Standard Labels .....	18	Note
<a href="#">PLAT722_ALERT_1_G</a>	Angle Calc 119.00, Rep 120.10 Dev...	1.10	Degree
	C32A -C33A -H33A 1 555 1 555 1 555 #	162	Check
<a href="#">PLAT779_ALERT_4_G</a>	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.60	Deg.
	C96 -CL62 -CL63 1 555 1 555 1 555 .....	#	489 Check
<a href="#">PLAT779_ALERT_4_G</a>	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	41.10	Deg.
	C96 -CL63 -CL62 1 555 1 555 1 555 .....	#	490 Check
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C1 (Sohnke SpGr)	S	Verify

## And 9 other PLAT791 Alerts

<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C1A (Sohnke SpGr)	S	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C2 (Sohnke SpGr)	S	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C2A (Sohnke SpGr)	S	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C3 (Sohnke SpGr)	S	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C3A (Sohnke SpGr)	R	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C4 (Sohnke SpGr)	R	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C4A (Sohnke SpGr)	R	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C5 (Sohnke SpGr)	R	Verify
<a href="#">PLAT791_ALERT_4_G</a>	Model has Chirality at C5A (Sohnke SpGr)	R	Verify
<a href="#">PLAT860_ALERT_3_G</a>	Number of Least-Squares Restraints .....	10	Note
<a href="#">PLAT933_ALERT_2_G</a>	Number of OMIT Records in Embedded .res File ...	25	Note

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
63 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  
46 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

## checkCIF publication errors

### Alert level A

<a href="#">PUBL004_ALERT_1_A</a>	The contact author's name and address are missing, _publ_contact_author_name and _publ_contact_author_address.
<a href="#">PUBL005_ALERT_1_A</a>	_publ_contact_author_email, _publ_contact_author_fax and _publ_contact_author_phone are all missing. At least one of these should be present.

- 2 **ALERT level A** = Data missing that is essential or data in wrong format  
0 **ALERT level G** = General alerts. Data that may be required is missing

### Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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. If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

#### Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

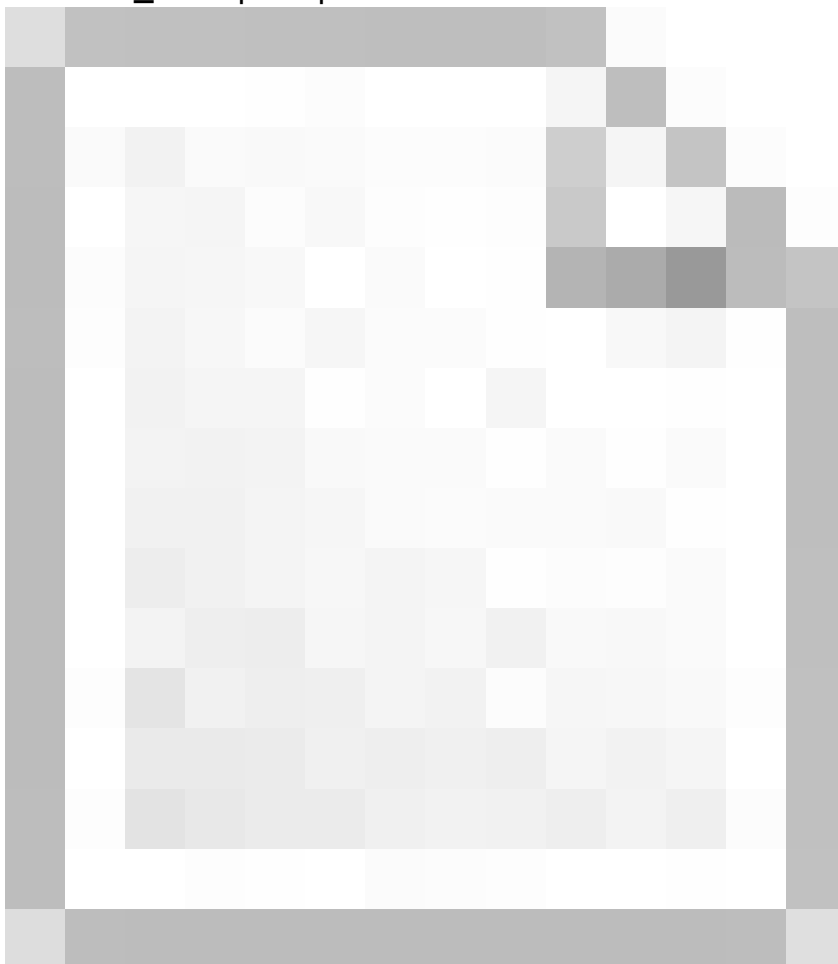
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If you wish to submit your CIF for publication in IUCrData you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

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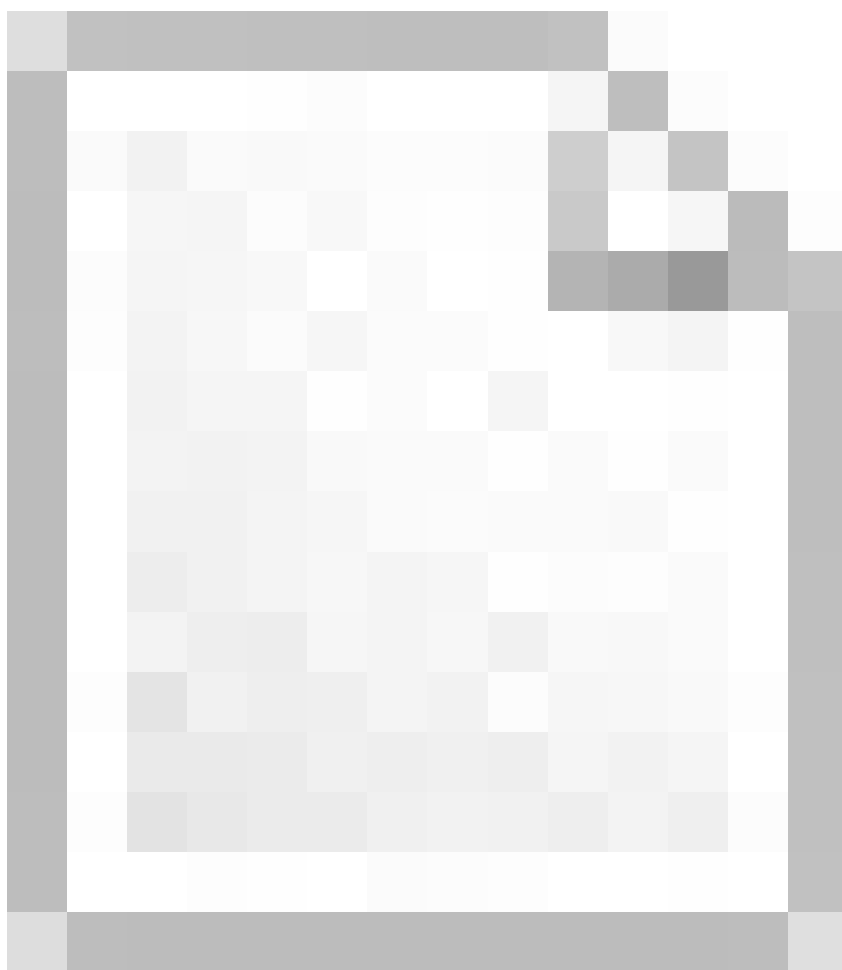
**PLATON version of 13/07/2021; check.def file version of 13/07/2021**

#### Datablock Ir\_2 - ellipsoid plot



#### Datablock Ru\_1 - ellipsoid plot





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