

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0190 Å Wavelength=1.54184

Cell: a=25.1943(5) b=25.1943(5) c=42.5843(7)
 alpha=90 beta=90 gamma=120
Temperature: 150 K

	Calculated	Reported
Volume	23409.1(12)	23409.1(10)
Space group	P 31 2 1	P 31 2 1
Hall group	P 31 2"	P 31 2"
Moiety formula	C220 H240 N6 O12 Ru6, 2(C H3) [+ solvent]	2(C66 H75 N3), 3 (C30 H32 O4 Ru2), 6 (C F3 S O3), 40 (C H4 O)
Sum formula	C222 H246 N6 O12 Ru6 [+ solvent]	C268 H418 F18 N6 O70 Ru6 S6
Mr	3796.68	5984.84
Dx, g cm ⁻³	0.808	1.274
Z	3	3
Mu (mm ⁻¹)	2.586	3.364
F000	5940.0	9450.0
F000'	5954.98	
h,k,lmax	31,31,52	30,30,51
Nref	31124[16665]	30645
Tmin,Tmax	0.466,0.590	0.784,1.000
Tmin'	0.394	

Correction method= # Reported T Limits: Tmin=0.784 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.98 Theta(max)= 72.812

R(reflections)= 0.0503(15980) wR2(reflections)= 0.1904(30645)

S = 0.945 Npar= 1107

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 3
From the CIF: _chemical_formula_weight 5984.84
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	222.00	2666.44
H	1.01	246.00	247.97
F	19.00	0.00	0.00
N	14.01	6.00	84.04
O	16.00	12.00	191.99
Ru	101.07	6.00	606.42
S	32.07	0.00	0.00

Calculated formula weight 3796.86

Author Response: The unit cell contains disordered methanol molecules which were not modelled but the corresponding scattering contribution were taken into account using SQUEEZE/PLATON procedure. The solvent composition (120 methanol molecules/cell) was included in the calculation of the empirical formula, molecular weight, density, linear absorption coefficient and F(000).

Alert level B

PLAT220_ALERT_2_B	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min)	Range	8.4	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	N3	--C41	..	8.4	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C59	--C60	..	7.2	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C65	--C66	..	19.0	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C68	--C69	..	9.0	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C75	--C76	..	8.0	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C92	--C93	..	10.3	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C93	--C94	..	7.3	s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C76	--	C81	0.30	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C77	--	C78	0.26	Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C84	--	C85	0.30	Ang.
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C65	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C93	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C96	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C103	Check	
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C107	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	Ru2	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	Ru3	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C57	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C92	Check	
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C104	Check	
PLAT369_ALERT_2_B	Long	C(sp2)-C(sp2) Bond	C102	- C107	1.59	Ang.
PLAT413_ALERT_2_B	Short	Inter XH3 .. XHn	H11	..H99C	1.91	Ang.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.447

From the CIF: _refine_ls_abs_structure_Flack_su 0.009

PLAT213_ALERT_2_C	Atom C98	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C102	has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C	Atom C107	has ADP max/min Ratio	3.1	prolat
PLAT213_ALERT_2_C	Atom C108	has ADP max/min Ratio	3.8	prolat
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	9.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C22	--C23 ..	5.7	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C38	--C39 ..	5.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C45	--C46 ..	5.7	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C63	--C64 ..	6.5	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C83	--C84 ..	6.9	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C98	--C99 ..	6.4	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C105	--C106 ..	7.0	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Ru1	-- C87	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Ru2	-- C97	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Ru3	-- C104	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O4	-- C81	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O6	-- C78	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N2	-- C28	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N2	-- C29	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N3	-- C40	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C3	-- C21	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C23	-- C24	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C26	-- C27	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C41	-- C42	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C60	-- C61	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C64	-- C65	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C67	-- C68	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C72	-- C73	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C72	-- C77	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C73	-- C74	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C79	-- C80	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C85	-- C86	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C88	-- C89	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C105	-- C109	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C109	-- C111	0.22	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C28	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C40	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C68	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C73	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C75	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C79	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C84	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C85	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C97	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C102	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Ru1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C26	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C42	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C45	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C53	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C61	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C64	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C69	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C72	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C74	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C76	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C77	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C80	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C88	Check

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C94	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C98	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C105	Check
PLAT334_ALERT_2_C	Small	Aver. Benzene C-C Dist C82 -C87	1.37	Ang.
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds	0.01898	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C57 - C58	1.36	Ang.
PLAT363_ALERT_2_C	Long	C(sp3)-C(sp2) Bond C95 - C98	1.68	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond C78 - C79	1.53	Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact H10 ..H55B	1.96	Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact H22 ..H59A	1.94	Ang.
PLAT905_ALERT_3_C	Negative	K value in the Analysis of Variance ...	-3.028	Report
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & Sth/L= 0.600	6	Report
PLAT978_ALERT_2_C	Number	C-C Bonds with Positive Residual Density.	0	Info

● Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and _chemical_formula_moiety. This is
 usually due to the moiety formula being in the wrong format.
 Atom count from _chemical_formula_sum: C268 H418 F18 N6 O70 Ru6 S6
 Atom count from _chemical_formula_moiety: C268 H406 F18 N6 O70 Ru6 S6

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C268 H418 F18 N6 O70 Ru6 S6
 Atom count from the _atom_site data: C222 H246 N6 O12 Ru6

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 3
 From the CIF: _chemical_formula_sum C268 H418 F18 N6 O70 Ru6 S6
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	804.00	666.00	138.00
H	1254.00	738.00	516.00
F	54.00	0.00	54.00
N	18.00	18.00	0.00
O	210.00	36.00	174.00
Ru	18.00	18.00	0.00
S	18.00	0.00	18.00

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 ...	16	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero	0.447	Note
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT044_ALERT_1_G	Calculated and Reported Density Dx Differ by ..	0.4660	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by ..	23.12	%
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2	Units
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	6	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	9	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru1 --O1	6.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru1 --O2	6.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru1 --C83	5.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru2 --N2	7.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ru3 --N3	7.7	s.u.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C67 -C71_a	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C69 -C69_a	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C72 -C77	1.42	Ang.

PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C76	-C81	1.44 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C72	-C77	0.19 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C76	-C81	0.19 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C82	-C87	0.20 Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C92 Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for		C101 Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C108 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11	..C99	3.14 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C23	..C107	3.18 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C92	..C101	1.76 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C93	..C101	2.47 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C97	..C101	2.94 Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		! Info
PLAT721_ALERT_1_G	Bond Calc 0.97000, Rep 0.96000 Dev...		0.01 Ang.
	C99 -H99A 1.555 1.555	# 235	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C92	--C101	1.76 Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		45 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		130 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		4 Note

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

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

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 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.

Datablock I - ellipsoid plot

