



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:33 PM GMT

PDB ID : 3P4C  
Title : Alternatingly modified 2'Fluoro RNA octamer f/rA2U2-R32  
Authors : Pallan, P.S.; Greene, E.M.; Jicman, P.A.; Pandey, R.K.; Manoharan, M.;  
Rozners, E.; Egli, M.  
Deposited on : 2010-10-06  
Resolution : 1.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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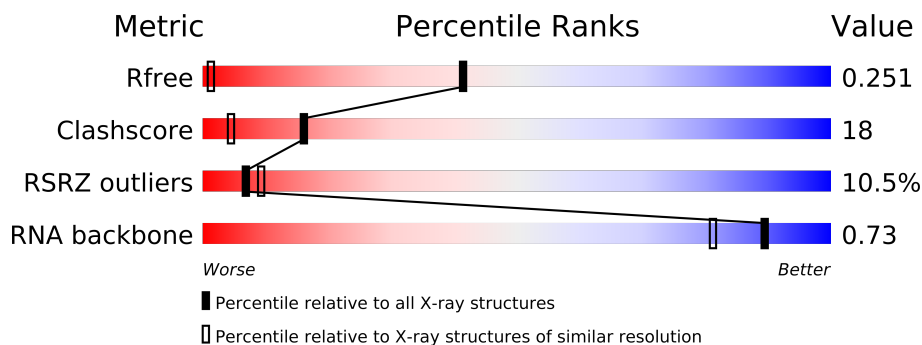
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1039 (1.20-1.08)
Clashscore	79885	1150 (1.20-1.08)
RSRZ outliers	66119	1039 (1.20-1.08)
RNA backbone	1838	1002 (2.92-0.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	8	
1	B	8	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SR	B	301	-	X
2	SR	B	302	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 452 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5'-R(\*(CFZ)P\*GP\*(AF2)P\*AP\*(UFT)P\*UP\*(CFZ)P\*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	8	Total	C	F	N	O	P	0	1	0
			189	86	4	35	57	7			
1	B	8	Total	C	F	N	O	P	0	0	0
			167	76	4	30	50	7			

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Sr	0	0
			3	3		

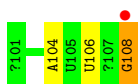
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	48	Total	O	0	0
			48	48		

i

● Molecule 1: 5'-R(\*<sub>1</sub>(CFZ)P\*<sub>2</sub>GP\*(AF2)P\*<sub>3</sub>AP\*(UFT)P\*<sub>4</sub>UP\*(CFZ)P\*<sub>5</sub>G)-3'

Chain A:



Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.55Å 40.55Å 117.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.15 30.12 – 1.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.15) 96.1 (30.12-1.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 1.15Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.182 , 0.249 0.178 , 0.251	Depositor DCC
$R_{free}$ test set	654 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 68.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 13343 reflections (0.022%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SR, CFZ, UFT, AF2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.79	4/121 (3.3%)	2.55	14/180 (7.8%)
1	B	1.34	1/96 (1.0%)	1.71	1/143 (0.7%)
All	All	1.60	5/217 (2.3%)	2.22	15/323 (4.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	U	C2'-O2'	8.06	1.52	1.41
1	A	104	A	C2'-O2'	-7.91	1.31	1.41
1	B	210	G	C2'-O2'	7.54	1.51	1.41
1	A	108[A]	G	C2'-O2'	5.57	1.48	1.41
1	A	108[B]	G	C2'-O2'	5.57	1.48	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108[A]	G	C5-C6-O6	-8.16	123.70	128.60
1	A	108[B]	G	C5-C6-O6	-8.16	123.70	128.60
1	A	108[A]	G	N3-C4-N9	7.54	130.52	126.00
1	A	108[B]	G	N3-C4-N9	7.54	130.52	126.00
1	A	108[A]	G	N3-C4-C5	-7.46	124.87	128.60
1	A	108[B]	G	N3-C4-C5	-7.46	124.87	128.60
1	A	104	A	N1-C2-N3	-6.68	125.96	129.30
1	B	212	A	N1-C2-N3	6.27	132.43	129.30
1	A	108[A]	G	C6-N1-C2	-5.61	121.73	125.10
1	A	108[B]	G	C6-N1-C2	-5.61	121.73	125.10
1	A	108[A]	G	C2-N3-C4	5.51	114.65	111.90
1	A	108[B]	G	C2-N3-C4	5.51	114.65	111.90
1	A	104	A	C5-N7-C8	5.18	106.49	103.90
1	A	108[A]	G	C5-C6-N1	5.15	114.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108[B]	G	C5-C6-N1	5.15	114.07	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	189	0	24	6	72
1	B	167	0	0	0	72
2	B	3	0	0	1	0
3	A	45	0	0	2	0
3	B	48	0	0	0	0
All	All	452	0	24	7	72

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108[B]:G:C2'	1:A:108[B]:G:O2'	1.67	1.39
3:A:355:HOH:O	2:B:302:SR:SR	1.80	0.70
1:A:108[B]:G:C1'	1:A:108[B]:G:O2'	2.44	0.64
1:A:108[B]:G:C3'	1:A:108[B]:G:O2'	2.42	0.63
1:A:108[B]:G:C2'	1:A:108[B]:G:HO2'	2.11	0.52
1:A:108[B]:G:N2	3:A:379:HOH:O	2.36	0.51
1:A:108[B]:G:H8	1:A:108[B]:G:O5'	2.01	0.43

All (72) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108[B]:G:N9	1:B:209:CFZ:C6[17_555]	0.38	1.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108[B]:G:C5	1:B:209:CFZ:C4[17_555]	0.50	1.70
1:A:108[B]:G:N7	1:B:209:CFZ:C5[17_555]	0.58	1.62
1:A:108[B]:G:N3	1:B:209:CFZ:C2[17_555]	0.65	1.55
1:A:108[B]:G:C4'	1:B:209:CFZ:C5'[17_555]	0.71	1.49
1:A:108[B]:G:C2	1:B:209:CFZ:O2[17_555]	0.79	1.41
1:A:108[B]:G:C1'	1:B:209:CFZ:O4'[17_555]	0.93	1.27
1:A:108[B]:G:C4	1:B:209:CFZ:N1[17_555]	0.93	1.27
1:A:108[B]:G:C6	1:B:209:CFZ:N3[17_555]	0.99	1.21
1:A:108[B]:G:C2'	1:B:209:CFZ:C3'[17_555]	1.02	1.18
1:A:108[B]:G:C8	1:B:209:CFZ:C5[17_555]	1.03	1.17
1:A:108[B]:G:C2	1:B:209:CFZ:C2[17_555]	1.07	1.13
1:A:108[B]:G:N3	1:B:209:CFZ:O2[17_555]	1.07	1.13
1:A:108[B]:G:N1	1:B:209:CFZ:N3[17_555]	1.08	1.12
1:A:108[B]:G:C3'	1:B:209:CFZ:O5'[17_555]	1.12	1.08
1:A:108[B]:G:C4	1:B:209:CFZ:C2[17_555]	1.12	1.08
1:A:108[B]:G:C6	1:B:209:CFZ:C4[17_555]	1.13	1.07
1:A:108[B]:G:C8	1:B:209:CFZ:C6[17_555]	1.15	1.05
1:A:108[B]:G:C5	1:B:209:CFZ:C5[17_555]	1.17	1.03
1:A:108[B]:G:N3	1:B:209:CFZ:N1[17_555]	1.17	1.03
1:A:108[B]:G:C4'	1:B:209:CFZ:O5'[17_555]	1.21	0.99
1:A:108[B]:G:O6	1:B:209:CFZ:N4[17_555]	1.21	0.99
1:A:108[B]:G:N2	1:B:209:CFZ:O2[17_555]	1.21	0.99
1:A:108[B]:G:C5	1:B:209:CFZ:N3[17_555]	1.22	0.98
1:A:108[B]:G:C4	1:B:209:CFZ:C6[17_555]	1.24	0.96
1:A:108[B]:G:N9	1:B:209:CFZ:N1[17_555]	1.25	0.95
1:A:108[B]:G:O2'	1:B:209:CFZ:C3'[17_555]	1.28	0.92
1:A:108[B]:G:O2'	1:B:209:CFZ:C4'[17_555]	1.30	0.90
1:A:108[B]:G:C3'	1:B:209:CFZ:C5'[17_555]	1.36	0.84
1:A:108[B]:G:N7	1:B:209:CFZ:C4[17_555]	1.45	0.75
1:A:108[B]:G:C2'	1:B:209:CFZ:C4'[17_555]	1.46	0.74
1:A:108[B]:G:O2'	1:B:209:CFZ:C2'[17_555]	1.51	0.69
1:A:108[B]:G:C1'	1:B:209:CFZ:C1'[17_555]	1.51	0.69
1:A:108[B]:G:C6	1:B:209:CFZ:N4[17_555]	1.51	0.69
1:A:108[B]:G:O4'	1:B:209:CFZ:O4'[17_555]	1.53	0.67
1:A:108[B]:G:C3'	1:B:209:CFZ:C4'[17_555]	1.53	0.67
1:A:108[B]:G:C4	1:B:209:CFZ:N3[17_555]	1.56	0.64
1:A:108[B]:G:C2'	1:B:209:CFZ:C2'[17_555]	1.60	0.60
1:A:108[B]:G:C3'	1:B:209:CFZ:C3'[17_555]	1.62	0.58
1:A:108[B]:G:C5'	1:B:209:CFZ:O5'[17_555]	1.63	0.57
1:A:108[B]:G:O2'	1:B:209:CFZ:F2'[17_555]	1.64	0.56
1:A:108[B]:G:C2	1:B:209:CFZ:N3[17_555]	1.66	0.54
1:A:108[B]:G:N9	1:B:209:CFZ:C5[17_555]	1.69	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108[B]:G:C2'	1:B:209:CFZ:O4'[17_555]	1.70	0.50
1:A:108[B]:G:O3'	1:B:209:CFZ:O3'[17_555]	1.72	0.48
1:A:108[B]:G:C4	1:B:209:CFZ:C5[17_555]	1.73	0.47
1:A:108[B]:G:C1'	1:B:209:CFZ:N1[17_555]	1.76	0.44
1:A:108[B]:G:N1	1:B:209:CFZ:C2[17_555]	1.78	0.42
1:A:108[B]:G:O4'	1:B:209:CFZ:C5'[17_555]	1.80	0.40
1:A:108[B]:G:C2'	1:B:209:CFZ:C1'[17_555]	1.80	0.40
1:A:108[B]:G:C5	1:B:209:CFZ:N4[17_555]	1.82	0.38
1:A:108[B]:G:C1'	1:B:209:CFZ:C6[17_555]	1.83	0.37
1:A:108[B]:G:C4	1:B:209:CFZ:C4[17_555]	1.85	0.35
1:A:108[B]:G:O2'	1:B:209:CFZ:O4'[17_555]	1.87	0.33
1:A:108[B]:G:O3'	1:B:209:CFZ:C5'[17_555]	1.88	0.32
1:A:108[B]:G:O3'	1:B:209:CFZ:C3'[17_555]	1.88	0.32
1:A:108[B]:G:C5	1:B:209:CFZ:C6[17_555]	1.88	0.32
1:A:108[B]:G:O3'	1:B:209:CFZ:C4'[17_555]	1.89	0.31
1:A:108[B]:G:N7	1:B:209:CFZ:C6[17_555]	1.89	0.31
1:A:108[B]:G:C4'	1:B:209:CFZ:C4'[17_555]	1.91	0.29
1:A:108[B]:G:C1'	1:B:209:CFZ:C4'[17_555]	1.92	0.28
1:A:108[B]:G:O2'	1:B:209:CFZ:O3'[17_555]	1.93	0.27
1:A:108[B]:G:O6	1:B:209:CFZ:C4[17_555]	1.93	0.27
1:A:108[B]:G:N3	1:B:209:CFZ:C1'[17_555]	1.93	0.27
1:A:108[B]:G:N3	1:B:209:CFZ:N3[17_555]	1.97	0.23
1:A:108[B]:G:O2'	1:B:209:CFZ:C1'[17_555]	1.99	0.21
1:A:108[B]:G:C5	1:B:209:CFZ:C2[17_555]	1.99	0.21
1:A:108[B]:G:O4'	1:B:209:CFZ:C4'[17_555]	2.00	0.20
1:A:108[B]:G:N7	1:B:209:CFZ:N4[17_555]	2.08	0.12
1:A:108[B]:G:O3'	1:B:209:CFZ:O5'[17_555]	2.10	0.10
1:A:108[B]:G:N1	1:B:209:CFZ:O2[17_555]	2.14	0.06
1:A:108[B]:G:C5'	1:B:209:CFZ:C5'[17_555]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2/8 (25%)	0	0
1	B	3/8 (37%)	0	0
All	All	5/16 (31%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CFZ	A	101	1	18,18,22	0.69	0	23,26,33	2.43	5 (21%)
1	AF2	A	103	1	22,24,25	0.91	0	32,35,38	1.33	5 (15%)
1	UFT	A	105	1	19,21,22	0.71	0	23,30,33	1.66	4 (17%)
1	CFZ	A	107	1	19,21,22	0.84	1 (5%)	24,30,33	1.46	4 (16%)
1	CFZ	B	209	1	18,18,22	0.88	0	23,26,33	2.12	7 (30%)
1	AF2	B	211	1	22,24,25	0.70	0	32,35,38	1.32	5 (15%)
1	UFT	B	213	1	19,21,22	0.97	1 (5%)	23,30,33	1.38	4 (17%)
1	CFZ	B	215	1	19,21,22	1.13	2 (10%)	24,30,33	1.54	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	101	1	-	0/4/22/26	0/2/2/2
1	AF2	A	103	1	-	0/8/25/26	0/1/3/3
1	UFT	A	105	1	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	107	1	-	0/6/25/26	0/2/2/2
1	CFZ	B	209	1	-	0/4/22/26	0/2/2/2
1	AF2	B	211	1	-	0/8/25/26	0/1/3/3
1	UFT	B	213	1	-	0/6/25/26	0/2/2/2
1	CFZ	B	215	1	-	0/6/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	CFZ	C2-N1	3.43	1.42	1.38
1	B	215	CFZ	P-O2P	2.54	1.49	1.46
1	A	107	CFZ	C2-N1	2.49	1.40	1.38
1	B	213	UFT	P-OP1	2.02	1.49	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	CFZ	C6-C5-C4	-8.57	113.91	117.47
1	B	209	CFZ	C2-N3-C4	6.19	124.53	115.57
1	A	101	CFZ	O5'-C5'-C4'	-4.84	106.50	113.28
1	A	105	UFT	C2-N1-C1'	-4.73	115.24	118.21
1	B	215	CFZ	C2-N3-C4	4.53	122.13	115.57
1	B	209	CFZ	C5-C6-N1	4.05	125.79	121.21
1	B	211	AF2	N3-C2-N1	-3.61	125.69	128.71
1	A	107	CFZ	C2-N1-C1'	-3.60	114.12	119.03
1	A	101	CFZ	C2-N3-C4	3.47	120.59	115.57
1	A	103	AF2	O4'-C1'-N9	-3.41	105.26	108.44
1	B	211	AF2	C5-C6-N6	3.20	127.95	120.72
1	A	105	UFT	C3'-C2'-C1'	-3.19	99.20	103.30
1	B	215	CFZ	C6-C5-C4	-3.14	116.17	117.47
1	B	211	AF2	N6-C6-N1	-3.05	113.38	119.36
1	B	213	UFT	C5-C6-N1	3.05	124.66	121.21
1	B	209	CFZ	N4-C4-N3	3.02	122.39	116.59
1	A	103	AF2	N3-C2-N1	-2.74	126.42	128.71
1	B	209	CFZ	C5-C4-N3	-2.67	118.08	121.68
1	A	107	CFZ	C3'-C2'-C1'	-2.47	100.12	103.30
1	A	101	CFZ	F2'-C2'-C1'	-2.46	103.78	109.61
1	A	107	CFZ	O4'-C1'-C2'	2.45	108.50	105.79
1	B	209	CFZ	O5'-C5'-C4'	-2.43	109.88	113.28
1	B	215	CFZ	C3'-C2'-C1'	-2.42	100.18	103.30
1	B	211	AF2	C3'-C2'-C1'	-2.42	100.19	103.30
1	A	103	AF2	C8-N9-C4	-2.41	105.06	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	CFZ	C6-C5-C4	-2.40	116.47	117.47
1	B	213	UFT	C5-C4-N3	-2.37	112.23	116.70
1	B	213	UFT	C6-N1-C1'	2.34	125.13	119.33
1	A	103	AF2	F-C2'-C1'	-2.30	104.16	109.61
1	B	209	CFZ	C6-N1-C1'	2.26	124.93	119.33
1	A	103	AF2	C8-N9-C1'	2.12	130.57	126.38
1	B	213	UFT	C3'-C2'-C1'	-2.12	100.57	103.30
1	A	105	UFT	C5-C6-N1	2.11	123.60	121.21
1	B	215	CFZ	C2-N1-C1'	-2.07	116.20	119.03
1	A	105	UFT	C6-N1-C1'	2.07	124.45	119.33
1	A	107	CFZ	C6-N1-C2	2.06	121.83	117.73
1	A	101	CFZ	C5-C6-N1	2.05	123.53	121.21
1	B	211	AF2	C8-N9-C4	-2.02	105.36	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	8/8 (100%)	0.19	1 (12%) 5 7	11, 13, 16, 17	0
1	B	8/8 (100%)	0.15	1 (12%) 5 7	8, 12, 17, 19	1 (12%)
All	All	16/16 (100%)	0.17	2 (12%) 7 7	8, 12, 17, 19	1 (6%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108[A]	G	3.4
1	B	209	CFZ	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	UFT	B	213	20/21	0.08	2.31	9,12,14,15	0
1	CFZ	A	101	17/21	0.09	0.61	11,14,22,24	0
1	UFT	A	105	20/21	0.07	0.27	10,12,16,18	0
1	CFZ	B	209	17/21	0.13	0.17	12,16,20,21	17
1	AF2	A	103	22/23	0.07	-0.47	8,10,12,16	0
1	AF2	B	211	22/23	0.07	-0.78	9,12,19,31	0
1	CFZ	B	215	20/21	0.06	-1.17	7,9,15,19	0
1	CFZ	A	107	20/21	0.06	-1.51	12,16,21,22	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SR	B	302	1/1	0.24	42.64	27,27,27,27	0
2	SR	B	301	1/1	0.21	2.31	19,19,19,19	0
2	SR	B	303	1/1	0.17	-	77,77,77,77	1

### 6.5 Other polymers ⓘ

There are no such residues in this entry.