



Full wwPDB X-ray Structure Validation Report

Nov 6, 2014 – 10:43 AM EST

PDB ID : 3P4A
Title : 2'Fluoro modified RNA octamer fA2U2
Authors : Manoharan, M.; Akinc, A.; Pandey, R.K.; Qin, J.; Hadwiger, P.; John, M.;
Mills, K.; Charisse, K.; Maier, M.A.; Nechev, L.; Greene, E.M.; Pallan, P.S.;
Rozners, E.; Rajeev, K.G.; Egli, M.
Deposited on : 2010-10-06
Resolution : 1.20 Å(reported)

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

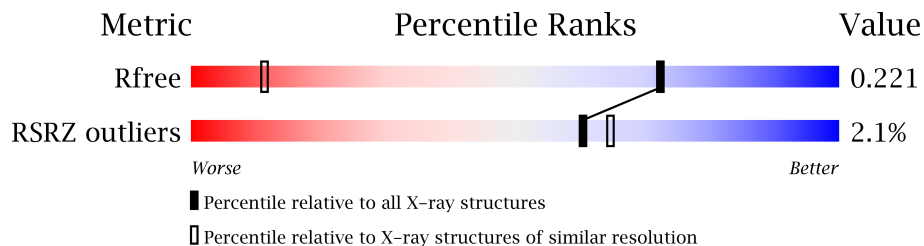
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 1.20 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	1038 (1.26-1.14)
RSRZ outliers	66119	1038 (1.26-1.14)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1404 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 2'Fluoro modified RNA 8-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	8	Total	C	F	N	O	P	0	0	0
			167	76	8	30	46	7			
1	B	8	Total	C	F	N	O	P	0	0	0
			167	76	8	30	46	7			
1	C	8	Total	C	F	N	O	P	0	2	0
			192	86	9	32	56	9			
1	D	8	Total	C	F	N	O	P	0	5	0
			237	106	11	40	69	11			
1	E	8	Total	C	F	N	O	P	0	0	0
			167	76	8	30	46	7			
1	F	8	Total	C	F	N	O	P	0	0	0
			167	76	8	30	46	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Sr	0	0
			2	2		
2	E	2	Total	Sr	0	0
			2	2		
2	B	1	Total	Sr	0	0
			1	1		
2	C	2	Total	Sr	0	0
			2	2		
2	A	1	Total	Sr	0	0
			1	1		
2	F	1	Total	Sr	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	50	Total 50	O 50	0	0
4	C	57	Total 57	O 57	0	0
4	D	53	Total 53	O 53	0	0
4	E	46	Total 46	O 46	0	0
4	F	51	Total 51	O 51	0	0

3 Residue-property plots

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4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	43.24Å 43.24Å 60.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.20 20.37 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.20) 96.2 (20.37-1.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.170 , 0.234 0.165 , 0.221	Depositor DCC
R_{free} test set	1929 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 88.9	EDS
Estimated twinning fraction	0.025 for -h,-k,l 0.487 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 39939 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1404	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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5.2 Close contacts ⓘ

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5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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5.3.2 Protein sidechains ⓘ

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5.3.3 RNA ⓘ

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

55 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	1.04	1 (5%)	23,26,33	1.49	3 (13%)
1	GF2	A	102	1	23,25,26	1.06	3 (13%)	32,37,40	5.91	8 (25%)
1	AF2	A	103	1	22,24,25	0.76	0	32,35,38	1.09	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AF2	A	104	1	22,24,25	0.87	0	32,35,38	1.28	2 (6%)
1	UFT	A	105	1	19,21,22	1.76	2 (10%)	23,30,33	1.45	3 (13%)
1	UFT	A	106	1	19,21,22	1.56	2 (10%)	23,30,33	1.34	3 (13%)
1	CFZ	A	107	1	19,21,22	0.94	0	24,30,33	1.31	3 (12%)
1	GF2	A	108	1,2	23,25,26	1.31	3 (13%)	32,37,40	3.62	2 (6%)
1	CFZ	B	209	1	18,18,22	1.27	3 (16%)	23,26,33	1.44	4 (17%)
1	GF2	B	210	1	23,25,26	1.37	2 (8%)	32,37,40	7.84	10 (31%)
1	AF2	B	211	1	22,24,25	0.82	1 (4%)	32,35,38	1.37	5 (15%)
1	AF2	B	212	1	22,24,25	0.86	1 (4%)	32,35,38	1.17	4 (12%)
1	UFT	B	213	1,2	19,21,22	1.54	2 (10%)	23,30,33	1.72	5 (21%)
1	UFT	B	214	1	19,21,22	1.28	1 (5%)	23,30,33	1.39	4 (17%)
1	CFZ	B	215	1	19,21,22	0.86	1 (5%)	24,30,33	1.58	5 (20%)
1	GF2	B	216	1	23,25,26	1.06	3 (13%)	32,37,40	2.99	6 (18%)
1	CFZ	C	301	1	18,18,22	1.11	2 (11%)	23,26,33	1.49	3 (13%)
1	GF2	C	302	1	23,25,26	0.98	2 (8%)	32,37,40	4.99	4 (12%)
1	AF2	C	303	1	22,24,25	0.87	0	32,35,38	0.93	1 (3%)
1	AF2	C	304	1	22,24,25	0.80	0	32,35,38	1.39	5 (15%)
1	UFT	C	305	1	19,21,22	1.99	2 (10%)	23,30,33	1.63	5 (21%)
1	UFT	C	306[A]	1	19,21,22	1.90	1 (5%)	23,30,33	1.69	6 (26%)
1	UFT	C	306[B]	1	19,21,22	1.55	1 (5%)	23,30,33	0.89	0
1	CFZ	C	307[A]	1	19,21,22	1.04	1 (5%)	24,30,33	1.40	3 (12%)
1	CFZ	C	307[B]	1	19,21,22	1.04	1 (5%)	24,30,33	1.45	3 (12%)
1	GF2	C	308	1	23,25,26	0.97	1 (4%)	32,37,40	3.87	2 (6%)
1	CFZ	D	409[A]	1	18,18,22	1.13	3 (16%)	23,26,33	1.39	3 (13%)
1	CFZ	D	409[B]	1	18,18,22	0.97	1 (5%)	23,26,33	1.21	4 (17%)
1	GF2	D	410[A]	1	23,25,26	1.10	1 (4%)	32,37,40	5.27	5 (15%)
1	GF2	D	410[B]	1	23,25,26	0.97	2 (8%)	32,37,40	5.96	5 (15%)
1	AF2	D	411[A]	1	22,24,25	0.93	2 (9%)	32,35,38	0.97	1 (3%)
1	AF2	D	411[B]	1	22,24,25	0.82	1 (4%)	32,35,38	1.07	2 (6%)
1	AF2	D	412	1	22,24,25	0.83	0	32,35,38	1.76	10 (31%)
1	UFT	D	413[A]	1	19,21,22	1.82	2 (10%)	23,30,33	1.55	5 (21%)
1	UFT	D	413[B]	1	19,21,22	1.49	1 (5%)	23,30,33	1.15	1 (4%)
1	UFT	D	414[A]	1	19,21,22	1.78	2 (10%)	23,30,33	2.10	6 (26%)
1	UFT	D	414[B]	1	19,21,22	1.80	2 (10%)	23,30,33	2.08	6 (26%)
1	CFZ	D	415	1	19,21,22	1.18	2 (10%)	24,30,33	1.43	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GF2	D	416	1	23,25,26	1.15	1 (4%)	32,37,40	4.33	5 (15%)
1	CFZ	E	501	1	18,18,22	1.12	3 (16%)	23,26,33	1.48	4 (17%)
1	GF2	E	502	1	23,25,26	1.45	2 (8%)	32,37,40	7.42	13 (40%)
1	AF2	E	503	1	22,24,25	0.89	1 (4%)	32,35,38	1.23	4 (12%)
1	AF2	E	504	1	22,24,25	0.89	0	32,35,38	1.17	2 (6%)
1	UFT	E	505	1,2	19,21,22	1.42	1 (5%)	23,30,33	1.34	2 (8%)
1	UFT	E	506	1	19,21,22	1.22	1 (5%)	23,30,33	1.66	4 (17%)
1	CFZ	E	507	1	19,21,22	0.97	2 (10%)	24,30,33	1.30	2 (8%)
1	GF2	E	508	1	23,25,26	0.99	2 (8%)	32,37,40	4.96	7 (21%)
1	CFZ	F	609	1	18,18,22	1.11	1 (5%)	23,26,33	1.12	1 (4%)
1	GF2	F	610	1	23,25,26	1.12	2 (8%)	32,37,40	4.63	5 (15%)
1	AF2	F	611	1	22,24,25	0.79	0	32,35,38	1.29	4 (12%)
1	AF2	F	612	1	22,24,25	0.82	0	32,35,38	1.53	5 (15%)
1	UFT	F	613	1	19,21,22	1.53	1 (5%)	23,30,33	1.86	4 (17%)
1	UFT	F	614	1	19,21,22	1.97	4 (21%)	23,30,33	1.35	3 (13%)
1	CFZ	F	615	1	19,21,22	0.92	0	24,30,33	1.55	3 (12%)
1	GF2	F	616	1,2	23,25,26	1.01	2 (8%)	32,37,40	4.94	4 (12%)

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	GF2	A	102	1	-	0/8/25/26	0/3/3/3
1	AF2	A	103	1	-	0/8/25/26	0/3/3/3
1	AF2	A	104	1	-	0/8/25/26	0/3/3/3
1	UFT	A	105	1	-	0/6/25/26	0/2/2/2
1	UFT	A	106	1	-	0/6/25/26	0/2/2/2
1	CFZ	A	107	1	-	0/6/25/26	0/2/2/2
1	GF2	A	108	1,2	-	0/8/25/26	0/3/3/3
1	CFZ	B	209	1	-	0/4/22/26	0/2/2/2
1	GF2	B	210	1	-	0/8/25/26	0/3/3/3
1	AF2	B	211	1	-	0/8/25/26	0/3/3/3
1	AF2	B	212	1	-	0/8/25/26	0/3/3/3
1	UFT	B	213	1,2	-	0/6/25/26	0/2/2/2
1	UFT	B	214	1	-	0/6/25/26	0/2/2/2
1	CFZ	B	215	1	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GF2	B	216	1	-	0/8/25/26	0/3/3/3
1	CFZ	C	301	1	-	0/4/22/26	0/2/2/2
1	GF2	C	302	1	-	0/8/25/26	0/3/3/3
1	AF2	C	303	1	-	0/8/25/26	0/3/3/3
1	AF2	C	304	1	-	0/8/25/26	0/3/3/3
1	UFT	C	305	1	-	0/6/25/26	0/2/2/2
1	UFT	C	306[A]	1	-	0/6/25/26	0/2/2/2
1	UFT	C	306[B]	1	-	0/6/25/26	0/2/2/2
1	CFZ	C	307[A]	1	-	0/6/25/26	0/2/2/2
1	CFZ	C	307[B]	1	-	0/6/25/26	0/2/2/2
1	GF2	C	308	1	-	0/8/25/26	0/3/3/3
1	CFZ	D	409[A]	1	-	0/4/22/26	0/2/2/2
1	CFZ	D	409[B]	1	-	0/4/22/26	0/2/2/2
1	GF2	D	410[A]	1	-	0/8/25/26	0/3/3/3
1	GF2	D	410[B]	1	-	0/8/25/26	0/3/3/3
1	AF2	D	411[A]	1	-	0/8/25/26	0/3/3/3
1	AF2	D	411[B]	1	-	0/8/25/26	0/3/3/3
1	AF2	D	412	1	-	0/8/25/26	0/3/3/3
1	UFT	D	413[A]	1	-	0/6/25/26	0/2/2/2
1	UFT	D	413[B]	1	-	0/6/25/26	0/2/2/2
1	UFT	D	414[A]	1	-	0/6/25/26	0/2/2/2
1	UFT	D	414[B]	1	-	0/6/25/26	0/2/2/2
1	CFZ	D	415	1	-	0/6/25/26	0/2/2/2
1	GF2	D	416	1	-	0/8/25/26	0/3/3/3
1	CFZ	E	501	1	-	0/4/22/26	0/2/2/2
1	GF2	E	502	1	-	0/8/25/26	0/3/3/3
1	AF2	E	503	1	-	0/8/25/26	0/3/3/3
1	AF2	E	504	1	-	0/8/25/26	0/3/3/3
1	UFT	E	505	1,2	-	0/6/25/26	0/2/2/2
1	UFT	E	506	1	-	0/6/25/26	0/2/2/2
1	CFZ	E	507	1	-	0/6/25/26	0/2/2/2
1	GF2	E	508	1	-	0/8/25/26	0/3/3/3
1	CFZ	F	609	1	-	0/4/22/26	0/2/2/2
1	GF2	F	610	1	-	0/8/25/26	0/3/3/3
1	AF2	F	611	1	-	0/8/25/26	0/3/3/3
1	AF2	F	612	1	-	0/8/25/26	0/3/3/3
1	UFT	F	613	1	-	0/6/25/26	0/2/2/2
1	UFT	F	614	1	-	0/6/25/26	0/2/2/2
1	CFZ	F	615	1	-	0/6/25/26	0/2/2/2
1	GF2	F	616	1,2	-	0/8/25/26	0/3/3/3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	305	UFT	C5-C4	7.41	1.45	1.37
1	C	306[A]	UFT	C5-C4	7.14	1.45	1.37
1	D	413[A]	UFT	C5-C4	6.88	1.45	1.37
1	F	614	UFT	C5-C4	6.78	1.44	1.37
1	D	414[A]	UFT	C5-C4	6.45	1.44	1.37
1	D	414[B]	UFT	C5-C4	6.45	1.44	1.37
1	A	105	UFT	C5-C4	6.44	1.44	1.37
1	C	306[B]	UFT	C5-C4	5.71	1.43	1.37
1	A	106	UFT	C5-C4	5.63	1.43	1.37
1	D	413[B]	UFT	C5-C4	5.46	1.43	1.37
1	F	613	UFT	C5-C4	5.43	1.43	1.37
1	B	213	UFT	C5-C4	5.17	1.43	1.37
1	E	502	GF2	O4'-C1'	4.95	1.47	1.41
1	E	505	UFT	C5-C4	4.73	1.42	1.37
1	B	214	UFT	C5-C4	4.35	1.42	1.37
1	E	506	UFT	C5-C4	4.29	1.42	1.37
1	B	210	GF2	O4'-C1'	4.25	1.46	1.41
1	B	209	CFZ	O2-C2	3.78	1.26	1.21
1	A	108	GF2	C6-N1	3.58	1.41	1.36
1	F	609	CFZ	C2-N1	3.48	1.42	1.38
1	C	308	GF2	O4'-C1'	3.23	1.45	1.41
1	D	416	GF2	O4'-C1'	3.21	1.45	1.41
1	F	614	UFT	O4'-C1'	3.16	1.45	1.41
1	D	414[A]	UFT	C6-C5	-2.84	1.31	1.38
1	D	414[B]	UFT	C6-C5	-2.84	1.31	1.38
1	A	105	UFT	C2-N1	2.84	1.41	1.38
1	F	610	GF2	C6-N1	2.68	1.40	1.36
1	D	409[A]	CFZ	O2-C2	2.61	1.25	1.21
1	E	502	GF2	C6-N1	2.61	1.40	1.36
1	F	616	GF2	C6-N1	2.60	1.40	1.36
1	A	101	CFZ	C2-N1	2.57	1.41	1.38
1	F	610	GF2	C5-N7	2.50	1.41	1.38
1	B	212	AF2	C8-N7	-2.50	1.29	1.34
1	D	410[A]	GF2	C6-N1	2.49	1.40	1.36
1	C	307[A]	CFZ	C2-N1	2.48	1.41	1.38
1	C	307[B]	CFZ	C2-N1	2.48	1.41	1.38
1	B	215	CFZ	C2-N1	2.48	1.41	1.38
1	A	108	GF2	C5-N7	2.45	1.41	1.38
1	F	614	UFT	C6-C5	-2.45	1.32	1.38
1	C	301	CFZ	O2-C2	2.43	1.25	1.21
1	E	507	CFZ	O2-C2	2.40	1.25	1.21
1	E	503	AF2	O4'-C1'	2.40	1.44	1.41
1	A	106	UFT	O4'-C1'	2.38	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	614	UFT	P-OP1	2.36	1.49	1.46
1	C	302	GF2	C6-N1	2.34	1.40	1.36
1	D	411[B]	AF2	C2-N3	2.31	1.36	1.32
1	D	411[A]	AF2	C2-N3	2.31	1.36	1.32
1	D	415	CFZ	C2-N1	2.31	1.40	1.38
1	F	616	GF2	C5-N7	2.30	1.40	1.38
1	E	507	CFZ	C2-N1	2.29	1.40	1.38
1	A	108	GF2	O4'-C1'	2.28	1.44	1.41
1	B	210	GF2	P-OP1	2.26	1.49	1.46
1	B	216	GF2	C8-N7	-2.22	1.30	1.34
1	B	216	GF2	C6-N1	2.22	1.39	1.36
1	D	411[A]	AF2	P-OP1	2.22	1.49	1.46
1	D	409[B]	CFZ	O2-C2	2.19	1.24	1.21
1	D	415	CFZ	O2-C2	2.19	1.24	1.21
1	E	501	CFZ	O2-C2	2.19	1.24	1.21
1	E	508	GF2	P-OP1	2.18	1.49	1.46
1	D	410[B]	GF2	C6-N1	2.17	1.39	1.36
1	D	413[A]	UFT	O4'-C1'	2.17	1.43	1.41
1	E	501	CFZ	O4'-C1'	2.15	1.43	1.41
1	D	409[A]	CFZ	O4'-C1'	2.13	1.43	1.41
1	B	211	AF2	O4'-C1'	2.12	1.43	1.41
1	E	501	CFZ	C6-C5	-2.12	1.33	1.38
1	A	102	GF2	C6-N1	2.12	1.39	1.36
1	D	409[A]	CFZ	C2-N1	2.10	1.40	1.38
1	C	301	CFZ	C2-N1	2.09	1.40	1.38
1	C	305	UFT	P-OP1	2.09	1.49	1.46
1	A	102	GF2	C2-N2	2.09	1.35	1.32
1	B	209	CFZ	C6-C5	-2.07	1.33	1.38
1	B	216	GF2	C5-N7	2.05	1.40	1.38
1	C	302	GF2	C8-N9	2.05	1.39	1.36
1	D	410[B]	GF2	C8-N7	-2.04	1.30	1.34
1	A	102	GF2	C5-N7	2.02	1.40	1.38
1	B	209	CFZ	O4'-C1'	2.02	1.43	1.41
1	E	508	GF2	C6-N1	2.01	1.39	1.36
1	B	213	UFT	P-OP1	2.00	1.49	1.46

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	GF2	C6-C5-N7	-43.06	128.34	134.14
1	E	502	GF2	C6-C5-N7	-40.27	128.72	134.14
1	D	410[B]	GF2	C6-C5-N7	-32.50	129.76	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GF2	C6-C5-N7	-31.98	129.83	134.14
1	D	410[A]	GF2	C6-C5-N7	-28.49	130.30	134.14
1	F	616	GF2	C6-C5-N7	-27.13	130.49	134.14
1	E	508	GF2	C6-C5-N7	-26.38	130.59	134.14
1	C	302	GF2	C6-C5-N7	-25.98	130.64	134.14
1	F	610	GF2	C6-C5-N7	-24.99	130.78	134.14
1	D	416	GF2	C6-C5-N7	-21.96	131.18	134.14
1	C	308	GF2	C6-C5-N7	-19.56	131.51	134.14
1	A	108	GF2	C6-C5-N7	-19.50	131.51	134.14
1	B	216	GF2	C6-C5-N7	-14.34	132.21	134.14
1	C	302	GF2	C6-N1-C2	9.62	125.63	120.20
1	D	416	GF2	C6-N1-C2	8.60	125.06	120.20
1	C	308	GF2	C6-N1-C2	8.00	124.72	120.20
1	D	410[B]	GF2	C6-N1-C2	7.05	124.18	120.20
1	F	613	UFT	C2-N1-C1'	-6.78	113.95	118.21
1	E	502	GF2	C6-N1-C2	6.28	123.75	120.20
1	B	210	GF2	C6-N1-C2	5.82	123.49	120.20
1	E	506	UFT	C2-N1-C1'	-5.74	114.61	118.21
1	A	102	GF2	C6-N1-C2	5.71	123.42	120.20
1	B	216	GF2	C6-N1-C2	5.70	123.42	120.20
1	D	410[A]	GF2	C6-N1-C2	5.65	123.39	120.20
1	E	508	GF2	C6-N1-C2	5.61	123.37	120.20
1	A	105	UFT	C2-N1-C1'	-4.96	115.10	118.21
1	D	414[A]	UFT	C2-N1-C1'	-4.95	115.10	118.21
1	D	414[B]	UFT	C2-N1-C1'	-4.95	115.10	118.21
1	D	412	AF2	C5-C4-N3	4.92	130.79	125.98
1	F	610	GF2	C6-N1-C2	4.46	122.72	120.20
1	C	301	CFZ	C2-N3-C4	4.42	122.01	115.65
1	B	213	UFT	N3-C2-N1	4.39	119.64	115.97
1	F	612	AF2	C8-N9-C4	-4.29	103.47	106.96
1	D	414[A]	UFT	C4'-O4'-C1'	-4.23	105.07	109.72
1	D	414[B]	UFT	C4'-O4'-C1'	-4.23	105.07	109.72
1	C	305	UFT	N3-C2-N1	-4.18	112.48	115.97
1	F	612	AF2	N3-C2-N1	-4.14	125.25	128.89
1	B	215	CFZ	C2-N3-C4	4.13	121.59	115.65
1	D	415	CFZ	C2-N3-C4	4.07	121.50	115.65
1	F	615	CFZ	C2-N3-C4	4.04	121.46	115.65
1	F	615	CFZ	C6-C5-C4	-4.03	115.59	117.51
1	D	414[A]	UFT	F2'-C2'-C1'	-3.85	100.35	109.64
1	D	414[B]	UFT	F2'-C2'-C1'	-3.85	100.35	109.64
1	A	101	CFZ	O5'-C5'-C4'	-3.79	107.97	113.35
1	C	307[A]	CFZ	C2-N3-C4	3.71	120.99	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307[B]	CFZ	C2-N3-C4	3.71	120.99	115.65
1	E	507	CFZ	C2-N3-C4	3.64	120.89	115.65
1	A	107	CFZ	C2-N3-C4	3.62	120.86	115.65
1	A	102	GF2	C2-N3-C4	-3.59	110.99	115.30
1	D	413[A]	UFT	N3-C2-N1	-3.58	112.98	115.97
1	A	104	AF2	N3-C2-N1	-3.54	125.78	128.89
1	A	101	CFZ	C6-C5-C4	-3.53	115.83	117.51
1	D	409[A]	CFZ	C2-N3-C4	3.50	120.69	115.65
1	B	214	UFT	C2-N1-C1'	-3.50	116.01	118.21
1	F	611	AF2	C2'-C1'-N9	-3.45	107.77	113.79
1	E	505	UFT	N3-C2-N1	3.41	118.82	115.97
1	E	502	GF2	O4'-C1'-C2'	3.38	109.59	105.82
1	F	616	GF2	C6-N1-C2	3.38	122.11	120.20
1	E	502	GF2	C3'-C2'-C1'	-3.35	98.98	103.30
1	B	210	GF2	C2-N3-C4	-3.35	111.28	115.30
1	D	410[A]	GF2	C3'-C2'-C1'	-3.28	99.08	103.30
1	B	213	UFT	C2-N1-C1'	-3.27	116.15	118.21
1	E	501	CFZ	O4'-C1'-C2'	3.27	109.46	105.82
1	E	501	CFZ	F2'-C2'-C1'	-3.26	101.76	109.64
1	B	209	CFZ	O5'-C5'-C4'	-3.23	108.76	113.35
1	D	413[A]	UFT	C2-N1-C1'	-3.23	116.18	118.21
1	B	209	CFZ	F2'-C2'-C1'	-3.20	101.91	109.64
1	A	106	UFT	F2'-C2'-C1'	-3.18	101.95	109.64
1	C	304	AF2	C5-C4-N3	3.18	129.08	125.98
1	E	507	CFZ	C3'-C2'-C1'	-3.17	99.22	103.30
1	E	502	GF2	C2'-C1'-N9	3.15	119.28	113.79
1	E	503	AF2	C5-C4-N3	3.13	129.04	125.98
1	E	502	GF2	C2-N3-C4	-3.11	111.58	115.30
1	B	215	CFZ	C3'-C2'-C1'	-3.10	99.31	103.30
1	D	412	AF2	C4-C5-N7	3.09	112.40	109.41
1	C	305	UFT	C2-N1-C1'	-3.06	116.29	118.21
1	B	210	GF2	C2'-C1'-N9	3.04	119.10	113.79
1	D	412	AF2	O4'-C1'-C2'	3.03	109.19	105.82
1	C	306[A]	UFT	C4'-O4'-C1'	-3.01	106.41	109.72
1	B	211	AF2	F-C2'-C1'	-3.01	102.37	109.64
1	F	610	GF2	N2-C2-N1	-3.01	114.59	117.82
1	E	504	AF2	C3'-C2'-C1'	-2.97	99.48	103.30
1	F	611	AF2	C8-N9-C4	-2.97	104.55	106.96
1	D	409[B]	CFZ	C2-N3-C4	2.96	119.90	115.65
1	F	611	AF2	C3'-C2'-C1'	-2.95	99.51	103.30
1	D	416	GF2	C2-N3-C4	-2.92	111.80	115.30
1	D	410[A]	GF2	C2-N3-C4	-2.92	111.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	609	CFZ	C2-N3-C4	2.91	119.84	115.65
1	F	612	AF2	C8-N9-C1'	2.89	131.60	126.15
1	D	411[B]	AF2	C3'-C2'-C1'	-2.88	99.59	103.30
1	D	411[A]	AF2	C3'-C2'-C1'	-2.88	99.59	103.30
1	B	212	AF2	C3'-C2'-C1'	-2.88	99.60	103.30
1	A	102	GF2	N1-C2-N3	2.87	125.66	121.78
1	C	306[A]	UFT	O4'-C1'-C2'	2.86	109.01	105.82
1	A	103	AF2	C3'-C2'-C1'	-2.86	99.61	103.30
1	E	508	GF2	C2'-C1'-N9	-2.85	108.81	113.79
1	E	508	GF2	C3'-C2'-C1'	-2.85	99.63	103.30
1	D	413[A]	UFT	O4'-C1'-C2'	2.85	108.99	105.82
1	A	106	UFT	C2-N1-C1'	-2.84	116.42	118.21
1	C	306[A]	UFT	P-O5'-C5'	-2.83	111.79	122.98
1	E	508	GF2	N1-C2-N3	2.82	125.59	121.78
1	D	412	AF2	C3'-C2'-C1'	-2.82	99.67	103.30
1	A	108	GF2	N1-C2-N3	2.82	125.59	121.78
1	F	614	UFT	C2-N1-C1'	-2.81	116.44	118.21
1	E	508	GF2	C2-N3-C4	-2.80	111.94	115.30
1	E	502	GF2	C4-C5-N7	2.80	112.11	109.41
1	B	215	CFZ	C6-C5-C4	-2.80	116.18	117.51
1	F	613	UFT	N3-C2-N1	-2.78	113.65	115.97
1	C	306[A]	UFT	C2-N1-C1'	-2.78	116.46	118.21
1	E	502	GF2	F-C2'-C1'	-2.77	102.95	109.64
1	B	216	GF2	C3'-C2'-C1'	-2.77	99.74	103.30
1	F	613	UFT	C3'-C2'-C1'	-2.77	99.74	103.30
1	A	101	CFZ	C2-N3-C4	2.76	119.62	115.65
1	D	416	GF2	C5-C4-N3	2.75	129.24	126.07
1	B	209	CFZ	C3'-C2'-C1'	-2.75	99.76	103.30
1	D	409[A]	CFZ	C3'-C2'-C1'	-2.73	99.78	103.30
1	B	216	GF2	C2-N3-C4	-2.73	112.03	115.30
1	B	211	AF2	C3'-C2'-C1'	-2.72	99.80	103.30
1	B	211	AF2	O4'-C1'-C2'	2.70	108.83	105.82
1	B	210	GF2	C3'-C2'-C1'	-2.70	99.83	103.30
1	E	503	AF2	F-C2'-C1'	-2.68	103.17	109.64
1	B	213	UFT	C6-N1-C1'	2.68	125.97	119.33
1	B	214	UFT	C6-C5-C4	2.68	122.13	117.18
1	C	305	UFT	O4'-C1'-C2'	2.66	108.78	105.82
1	B	213	UFT	C6-C5-C4	2.65	122.09	117.18
1	B	212	AF2	C5-C6-N6	2.65	126.71	120.72
1	D	414[A]	UFT	C2'-C3'-C4'	-2.63	98.03	102.10
1	D	414[B]	UFT	C2'-C3'-C4'	-2.63	98.03	102.10
1	C	303	AF2	C3'-C2'-C1'	-2.61	99.95	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	CFZ	C3'-C2'-C1'	-2.60	99.95	103.30
1	F	614	UFT	C3'-C2'-C1'	-2.60	99.95	103.30
1	B	213	UFT	F2'-C2'-C1'	-2.59	103.38	109.64
1	E	502	GF2	C4'-O4'-C1'	-2.59	106.87	109.72
1	D	412	AF2	C4'-O4'-C1'	-2.58	106.88	109.72
1	E	505	UFT	C6-N1-C1'	2.57	125.71	119.33
1	A	104	AF2	C4-C5-N7	2.57	111.89	109.41
1	E	501	CFZ	C2-N3-C4	2.56	119.34	115.65
1	C	302	GF2	C3'-C2'-C1'	-2.56	100.00	103.30
1	B	216	GF2	C2'-C1'-N9	-2.55	109.34	113.79
1	C	301	CFZ	F2'-C2'-C1'	-2.52	103.54	109.64
1	C	304	AF2	C3'-C2'-C1'	-2.50	100.08	103.30
1	E	501	CFZ	C3'-C2'-C1'	-2.49	100.09	103.30
1	F	616	GF2	N1-C2-N3	2.48	125.13	121.78
1	D	410[B]	GF2	C3'-C2'-C1'	-2.48	100.11	103.30
1	E	506	UFT	C6-N1-C2	2.48	122.96	119.51
1	D	414[A]	UFT	N3-C2-N1	-2.47	113.91	115.97
1	D	414[B]	UFT	N3-C2-N1	-2.47	113.91	115.97
1	D	409[B]	CFZ	O5'-C5'-C4'	-2.47	109.84	113.35
1	C	304	AF2	C8-N9-C4	-2.47	104.95	106.96
1	F	610	GF2	C3'-C2'-C1'	-2.45	100.15	103.30
1	B	215	CFZ	C2-N1-C1'	-2.44	115.71	119.03
1	A	103	AF2	C2'-C1'-N9	-2.43	109.55	113.79
1	D	410[A]	GF2	N1-C2-N3	2.43	125.06	121.78
1	D	411[B]	AF2	P-O5'-C5'	-2.41	113.47	122.98
1	A	107	CFZ	C3'-C2'-C1'	-2.40	100.21	103.30
1	B	216	GF2	N1-C2-N3	2.40	125.02	121.78
1	E	502	GF2	O4'-C1'-N9	-2.40	102.88	108.10
1	E	502	GF2	C5-C4-N9	-2.39	103.77	107.09
1	A	106	UFT	C3'-C2'-C1'	-2.39	100.22	103.30
1	D	412	AF2	C2'-C1'-N9	-2.39	109.62	113.79
1	F	615	CFZ	C3'-C2'-C1'	-2.37	100.25	103.30
1	F	616	GF2	C2-N3-C4	-2.37	112.46	115.30
1	C	306[A]	UFT	C6-N1-C2	2.35	122.78	119.51
1	C	304	AF2	C4-C5-N7	2.35	111.68	109.41
1	D	413[B]	UFT	N3-C2-N1	-2.34	114.02	115.97
1	D	412	AF2	C6-C5-C4	-2.32	114.94	117.55
1	C	306[A]	UFT	O3'-C3'-C2'	2.31	119.25	112.15
1	B	215	CFZ	O4'-C1'-C2'	2.30	108.39	105.82
1	D	412	AF2	N6-C6-N1	2.30	123.99	119.11
1	F	614	UFT	F2'-C2'-C1'	-2.30	104.09	109.64
1	B	210	GF2	N1-C2-N3	2.30	124.88	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	409[B]	CFZ	O4'-C1'-C2'	2.29	108.37	105.82
1	F	611	AF2	O4'-C1'-C2'	2.29	108.37	105.82
1	E	502	GF2	C5-C4-N3	2.29	128.70	126.07
1	A	102	GF2	C2'-C1'-N9	-2.28	109.80	113.79
1	B	214	UFT	C3'-C2'-C1'	-2.28	100.36	103.30
1	E	504	AF2	C8-N9-C1'	2.27	130.43	126.15
1	B	211	AF2	N3-C2-N1	-2.28	126.89	128.89
1	A	102	GF2	N2-C2-N1	-2.26	115.39	117.82
1	E	506	UFT	F2'-C2'-C1'	-2.26	104.18	109.64
1	D	416	GF2	F-C2'-C1'	-2.25	104.20	109.64
1	E	503	AF2	O4'-C1'-C2'	2.25	108.32	105.82
1	B	210	GF2	F-C2'-C1'	-2.25	104.21	109.64
1	B	210	GF2	O4'-C1'-C2'	2.24	108.32	105.82
1	C	307[A]	CFZ	F2'-C2'-C1'	-2.24	104.22	109.64
1	C	307[B]	CFZ	F2'-C2'-C1'	-2.24	104.22	109.64
1	F	612	AF2	N7-C8-N9	2.24	117.28	112.20
1	B	212	AF2	C5-C4-N3	2.22	128.15	125.98
1	B	214	UFT	F2'-C2'-C1'	-2.22	104.29	109.64
1	A	102	GF2	C3'-C2'-C1'	-2.21	100.45	103.30
1	B	210	GF2	O4'-C1'-N9	-2.20	103.31	108.10
1	E	503	AF2	C3'-C2'-C1'	-2.19	100.47	103.30
1	D	410[B]	GF2	C2-N3-C4	-2.17	112.69	115.30
1	A	105	UFT	C3'-C2'-C1'	-2.17	100.50	103.30
1	D	412	AF2	C8-N9-C1'	2.16	130.22	126.15
1	D	413[A]	UFT	C3'-C2'-C1'	-2.16	100.52	103.30
1	C	304	AF2	O4'-C1'-C2'	2.15	108.22	105.82
1	A	102	GF2	C5-C4-N3	2.14	128.53	126.07
1	E	506	UFT	C3'-C2'-C1'	-2.13	100.55	103.30
1	B	209	CFZ	O4'-C1'-C2'	2.13	108.19	105.82
1	C	307[A]	CFZ	C6-N1-C1'	2.12	124.59	119.33
1	C	307[B]	CFZ	C6-N1-C1'	2.12	124.59	119.33
1	D	414[A]	UFT	F2'-C2'-C3'	-2.12	103.95	109.22
1	D	414[B]	UFT	F2'-C2'-C3'	-2.12	103.95	109.22
1	D	413[A]	UFT	C6-N1-C2	2.10	122.43	119.51
1	C	305	UFT	C3'-C2'-C1'	-2.09	100.60	103.30
1	D	410[B]	GF2	N2-C2-N1	-2.08	115.59	117.82
1	C	305	UFT	C6-N1-C2	2.08	122.42	119.51
1	D	412	AF2	C2-N3-C4	-2.08	107.27	113.27
1	D	409[B]	CFZ	C3'-C2'-C1'	-2.08	100.62	103.30
1	E	502	GF2	N1-C2-N3	2.07	124.58	121.78
1	A	103	AF2	C5-C6-N6	2.07	125.41	120.72
1	E	508	GF2	C6-C5-C4	2.07	120.53	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	610	GF2	N1-C2-N3	2.07	124.57	121.78
1	D	409[A]	CFZ	O5'-C5'-C4'	-2.06	110.42	113.35
1	C	302	GF2	C5-C4-N3	2.05	128.43	126.07
1	B	212	AF2	C2'-C1'-N9	-2.05	110.22	113.79
1	B	210	GF2	C4-C5-N7	2.04	111.38	109.41
1	F	612	AF2	O4'-C1'-C2'	2.04	108.10	105.82
1	A	105	UFT	N3-C2-N1	-2.04	114.27	115.97
1	A	107	CFZ	C6-N1-C1'	2.02	124.33	119.33
1	B	211	AF2	C1'-N9-C4	-2.01	123.17	126.64
1	F	613	UFT	C6-N1-C2	2.00	122.30	119.51

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 11 ligands modelled in this entry, 11 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, 95th 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 ²)	Q<0.9
1	A	8/8 (100%)	-0.48	0 100 100	10, 13, 18, 26	0
1	B	8/8 (100%)	-0.28	0 100 100	12, 14, 16, 18	0
1	C	8/8 (100%)	0.02	0 100 100	10, 12, 19, 22	0
1	D	8/8 (100%)	0.64	1 (12%) 5 5	10, 12, 19, 23	0
1	E	8/8 (100%)	-0.06	0 100 100	12, 14, 16, 19	0
1	F	8/8 (100%)	-0.20	0 100 100	10, 13, 18, 24	0
All	All	48/48 (100%)	-0.06	1 (2%) 60 65	10, 14, 22, 26	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	416	GF2	2.0

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, 95th 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 ²)	Q<0.9
1	GF2	F	616	23/24	0.06	-	8,9,13,15	0
1	GF2	D	410[A]	23/24	0.08	-	8,9,9,10	23
1	UFT	F	614	20/21	0.06	-	11,12,18,18	0
1	AF2	E	504	22/23	0.07	-	10,13,17,20	0
1	GF2	D	410[B]	23/24	0.08	-	7,9,14,16	23
1	AF2	C	303	22/23	0.07	-	9,10,12,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	GF2	F	610	23/24	0.08	-	12,15,24,31	0
1	CFZ	F	615	20/21	0.07	-	9,11,14,17	0
1	GF2	B	216	23/24	0.08	-	15,17,20,22	0
1	CFZ	D	415	20/21	0.09	-	10,15,27,31	0
1	UFT	C	306[A]	20/21	0.12	-	16,20,28,29	20
1	UFT	B	213	20/21	0.07	-	13,16,19,20	0
1	AF2	D	412	22/23	0.07	-	11,15,22,23	0
1	UFT	C	306[B]	20/21	0.12	-	16,21,30,31	20
1	UFT	E	505	20/21	0.09	-	14,16,19,19	0
1	CFZ	A	107	20/21	0.07	-	9,12,15,17	0
1	UFT	A	106	20/21	0.07	-	10,12,18,19	0
1	UFT	F	613	20/21	0.06	-	9,11,20,21	0
1	UFT	B	214	20/21	0.09	-	13,15,21,23	0
1	AF2	F	611	22/23	0.08	-	12,14,18,22	0
1	CFZ	C	307[A]	20/21	0.10	-	10,15,26,26	5
1	CFZ	B	209	17/21	0.07	-	10,12,16,19	0
1	CFZ	F	609	17/21	0.08	-	19,22,27,35	0
1	UFT	E	506	20/21	0.09	-	13,14,23,24	0
1	UFT	D	414[A]	20/21	0.11	-	17,22,27,29	0
1	CFZ	C	307[B]	20/21	0.10	-	10,15,27,30	5
1	CFZ	E	501	17/21	0.08	-	10,12,15,19	0
1	UFT	A	105	20/21	0.07	-	10,11,20,21	0
1	CFZ	D	409[B]	17/21	0.08	-	8,11,18,18	17
1	GF2	A	108	23/24	0.06	-	8,9,12,14	0
1	UFT	D	414[B]	20/21	0.11	-	17,22,26,35	5
1	CFZ	D	409[A]	17/21	0.08	-	9,10,12,13	17
1	AF2	D	411[B]	22/23	0.07	-	8,10,15,15	5
1	CFZ	C	301	17/21	0.06	-	9,10,13,15	0
1	GF2	E	502	23/24	0.07	-	9,11,14,16	0
1	GF2	A	102	23/24	0.07	-	13,15,24,27	0
1	AF2	D	411[A]	22/23	0.07	-	8,10,11,12	5
1	UFT	C	305	20/21	0.08	-	12,18,27,27	0
1	AF2	E	503	22/23	0.08	-	11,12,14,16	0
1	GF2	C	308	23/24	0.08	-	8,11,18,21	0
1	CFZ	A	101	17/21	0.08	-	19,23,33,51	0
1	CFZ	B	215	20/21	0.07	-	12,14,16,17	0
1	GF2	D	416	23/24	0.09	-	9,11,17,22	0
1	AF2	B	211	22/23	0.07	-	10,12,14,16	0
1	GF2	C	302	23/24	0.07	-	8,9,11,11	0
1	UFT	D	413[B]	20/21	0.10	-	13,20,28,29	20
1	GF2	B	210	23/24	0.08	-	9,12,14,16	0
1	GF2	E	508	23/24	0.07	-	16,17,21,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	UFT	D	413[A]	20/21	0.10	-	11,18,25,25	20
1	AF2	A	104	22/23	0.09	-	11,13,17,21	0
1	AF2	A	103	22/23	0.07	-	12,15,18,23	0
1	AF2	B	212	22/23	0.07	-	10,13,17,18	0
1	CFZ	E	507	20/21	0.07	-	11,14,16,16	0
1	AF2	C	304	22/23	0.07	-	11,16,24,27	0
1	AF2	F	612	22/23	0.09	-	11,14,17,22	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, 95th 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(\AA^2)	Q<0.9
2	SR	E	703	1/1	0.13	-	18,18,18,18	1
2	SR	D	702	1/1	0.21	-	20,20,20,20	0
2	SR	F	706	1/1	0.26	-	18,18,18,18	1
2	SR	D	708	1/1	0.20	-	23,23,23,23	0
3	MG	E	712	1/1	0.29	-	21,21,21,21	1
2	SR	C	701	1/1	0.22	-	21,21,21,21	0
2	SR	A	705	1/1	0.22	-	32,32,32,32	0
2	SR	E	709	1/1	0.16	-	28,28,28,28	1
2	SR	B	704	1/1	0.13	-	18,18,18,18	1
3	MG	B	711	1/1	0.29	-	19,19,19,19	1
2	SR	C	707	1/1	0.21	-	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.