



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:32 AM GMT

PDB ID : 3P4A  
Title : 2'Fluoro modified RNA octamer fA2U2  
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Deposited on : 2010-10-06  
Resolution : 1.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

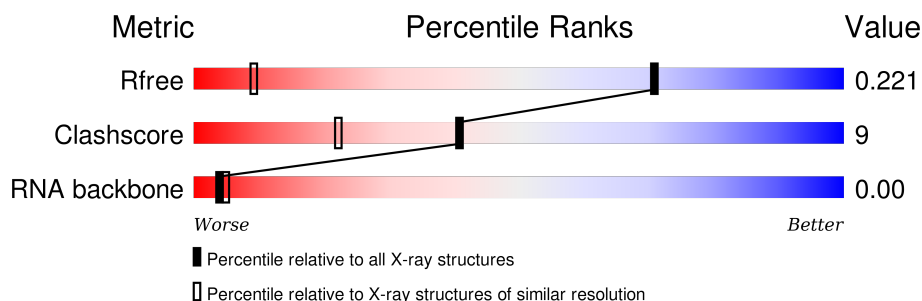
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






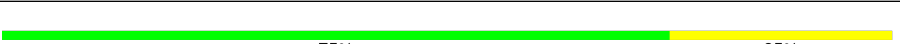
The reported resolution of this entry is 1.20 Å.

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))
$R_{free}$	91344	1495 (1.26-1.14)
Clashscore	102246	1607 (1.26-1.14)
RNA backbone	2183	1046 (2.70-0.62)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	8	
1	B	8	
1	C	8	
1	D	8	
1	E	8	
1	F	8	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

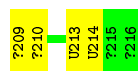
- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain A: 



- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain B: 



- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain C: 



- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain D: 



- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain E: 



- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.24 Å 43.24 Å 60.79 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 1.20 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.170 , 0.234 0.165 , 0.221	Depositor DCC
$R_{free}$ test set	1986 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.2	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 66.6	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 <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: MG, GF2, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	167	0	79	1	0
1	B	167	0	79	3	0
1	C	192	0	84	2	0
1	D	237	0	101	4	0
1	E	167	0	79	2	0
1	F	167	0	79	1	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	1	0
2	F	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
4	A	39	0	0	0	0
4	B	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	57	0	0	0	0
4	D	53	0	0	0	0
4	E	46	0	0	1	0
4	F	51	0	0	0	0
All	All	1404	0	501	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306[B]:UFT:H6	1:C:306[B]:UFT:H5'A	1.72	0.70
1:D:409[B]:CFZ:H2'	1:D:410[B]:GF2:H8	1.79	0.65
2:E:709:SR:SR	4:E:922:HOH:O	1.89	0.61
1:E:501:CFZ:H2'	1:E:502:GF2:H8	1.86	0.58
1:B:213:UFT:H2'	1:B:214:UFT:H6	1.84	0.58
1:B:209:CFZ:H2'	1:B:210:GF2:H8	1.87	0.55
1:C:301:CFZ:H2'	1:C:302:GF2:H8	1.93	0.50
1:A:104:AF2:H2'	1:A:105:UFT:H6	1.96	0.47
1:B:213:UFT:H2'	1:B:214:UFT:C6	2.47	0.45
1:D:409[B]:CFZ:H2'	1:D:410[B]:GF2:C8	2.46	0.44
1:E:505:UFT:H2'	1:E:506:UFT:H6	1.99	0.43
1:D:409[A]:CFZ:H2'	1:D:410[A]:GF2:H8	2.01	0.42
1:F:612:AF2:H2'	1:F:613:UFT:H6	2.00	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/8	-	-
1	B	0/8	-	-
1	C	0/8	-	-
1	D	0/8	-	-
1	E	0/8	-	-
1	F	0/8	-	-
All	All	0/48	-	-

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 ⓘ

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	14,18,22	0.84	0	18,26,33	1.13	1 (5%)
1	GF2	A	102	1	17,25,26	1.22	2 (11%)	20,37,40	2.46	3 (15%)
1	AF2	A	103	1	16,24,25	0.66	0	17,35,38	1.01	1 (5%)
1	AF2	A	104	1	16,24,25	0.88	1 (6%)	17,35,38	1.49	2 (11%)
1	UFT	A	105	1	12,21,22	1.05	1 (8%)	17,30,33	3.37	2 (11%)
1	UFT	A	106	1	12,21,22	1.27	2 (16%)	17,30,33	3.31	3 (17%)
1	CFZ	A	107	1	13,21,22	0.90	0	18,30,33	1.28	2 (11%)
1	GF2	A	108	1,2	17,25,26	1.53	2 (11%)	20,37,40	2.05	2 (10%)
1	CFZ	B	209	1	14,18,22	0.97	2 (14%)	18,26,33	1.11	2 (11%)
1	GF2	B	210	1	17,25,26	1.59	2 (11%)	20,37,40	2.67	7 (35%)
1	AF2	B	211	1	16,24,25	0.85	1 (6%)	17,35,38	1.55	4 (23%)
1	AF2	B	212	1	16,24,25	0.91	1 (6%)	17,35,38	0.95	0
1	UFT	B	213	1,2	12,21,22	1.20	1 (8%)	17,30,33	2.73	5 (29%)
1	UFT	B	214	1	12,21,22	1.19	1 (8%)	17,30,33	3.06	4 (23%)
1	CFZ	B	215	1	13,21,22	0.45	0	18,30,33	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GF2	B	216	1	17,25,26	1.23	2 (11%)	20,37,40	2.41	3 (15%)
1	CFZ	C	301	1	14,18,22	0.90	0	18,26,33	1.46	2 (11%)
1	GF2	C	302	1	17,25,26	1.18	1 (5%)	20,37,40	2.71	4 (20%)
1	AF2	C	303	1	16,24,25	0.82	0	17,35,38	0.90	0
1	AF2	C	304	1	16,24,25	0.76	0	17,35,38	1.28	3 (17%)
1	UFT	C	305	1	12,21,22	1.33	2 (16%)	17,30,33	3.87	3 (17%)
1	UFT	C	306[A]	1	12,21,22	1.29	2 (16%)	17,30,33	3.19	5 (29%)
1	UFT	C	306[B]	1	12,21,22	1.18	1 (8%)	17,30,33	3.23	2 (11%)
1	CFZ	C	307[A]	1	13,21,22	0.90	0	18,30,33	1.41	2 (11%)
1	CFZ	C	307[B]	1	13,21,22	0.90	0	18,30,33	1.44	2 (11%)
1	GF2	C	308	1	17,25,26	1.22	2 (11%)	20,37,40	2.61	3 (15%)
1	CFZ	D	409[A]	1	14,18,22	0.92	1 (7%)	18,26,33	1.29	1 (5%)
1	CFZ	D	409[B]	1	14,18,22	0.78	0	18,26,33	1.09	2 (11%)
1	GF2	D	410[A]	1	17,25,26	1.28	1 (5%)	20,37,40	2.33	2 (10%)
1	GF2	D	410[B]	1	17,25,26	1.17	2 (11%)	20,37,40	2.47	3 (15%)
1	AF2	D	411[A]	1	16,24,25	0.84	1 (6%)	17,35,38	0.87	0
1	AF2	D	411[B]	1	16,24,25	0.84	1 (6%)	17,35,38	0.89	0
1	AF2	D	412	1	16,24,25	0.80	0	17,35,38	1.64	6 (35%)
1	UFT	D	413[A]	1	12,21,22	1.30	2 (16%)	17,30,33	3.73	3 (17%)
1	UFT	D	413[B]	1	12,21,22	1.21	1 (8%)	17,30,33	3.42	2 (11%)
1	UFT	D	414[A]	1	12,21,22	1.29	2 (16%)	17,30,33	3.68	5 (29%)
1	UFT	D	414[B]	1	12,21,22	1.29	2 (16%)	17,30,33	3.67	5 (29%)
1	CFZ	D	415	1	13,21,22	0.99	0	18,30,33	1.42	1 (5%)
1	GF2	D	416	1	17,25,26	1.38	2 (11%)	20,37,40	2.69	4 (20%)
1	CFZ	E	501	1	14,18,22	1.06	2 (14%)	18,26,33	1.40	3 (16%)
1	GF2	E	502	1	17,25,26	1.77	3 (17%)	20,37,40	2.85	8 (40%)
1	AF2	E	503	1	16,24,25	0.87	1 (6%)	17,35,38	1.17	2 (11%)
1	AF2	E	504	1	16,24,25	0.82	0	17,35,38	0.94	0
1	UFT	E	505	1,2	12,21,22	1.19	1 (8%)	17,30,33	2.79	3 (17%)
1	UFT	E	506	1	12,21,22	1.03	1 (8%)	17,30,33	3.07	3 (17%)
1	CFZ	E	507	1	13,21,22	0.65	0	18,30,33	1.20	1 (5%)
1	GF2	E	508	1	17,25,26	1.19	1 (5%)	20,37,40	2.53	3 (15%)
1	CFZ	F	609	1	14,18,22	0.67	0	18,26,33	1.03	1 (5%)
1	GF2	F	610	1	17,25,26	1.28	1 (5%)	20,37,40	2.29	3 (15%)
1	AF2	F	611	1	16,24,25	0.77	0	17,35,38	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AF2	F	612	1	16,24,25	0.92	0	17,35,38	1.54	1 (5%)
1	UFT	F	613	1	12,21,22	1.18	1 (8%)	17,30,33	3.33	2 (11%)
1	UFT	F	614	1	12,21,22	1.49	3 (25%)	17,30,33	3.38	3 (17%)
1	CFZ	F	615	1	13,21,22	0.85	0	18,30,33	1.30	1 (5%)
1	GF2	F	616	1,2	17,25,26	1.27	1 (5%)	20,37,40	2.11	2 (10%)

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	-	0/2/22/26	0/2/2/2
1	GF2	A	102	1	-	0/3/25/26	0/3/3/3
1	AF2	A	103	1	-	0/3/25/26	0/3/3/3
1	AF2	A	104	1	-	0/3/25/26	0/3/3/3
1	UFT	A	105	1	-	0/3/25/26	0/2/2/2
1	UFT	A	106	1	-	0/3/25/26	0/2/2/2
1	CFZ	A	107	1	-	0/3/25/26	0/2/2/2
1	GF2	A	108	1,2	-	0/3/25/26	0/3/3/3
1	CFZ	B	209	1	-	0/2/22/26	0/2/2/2
1	GF2	B	210	1	-	0/3/25/26	0/3/3/3
1	AF2	B	211	1	-	0/3/25/26	0/3/3/3
1	AF2	B	212	1	-	0/3/25/26	0/3/3/3
1	UFT	B	213	1,2	-	0/3/25/26	0/2/2/2
1	UFT	B	214	1	-	0/3/25/26	0/2/2/2
1	CFZ	B	215	1	-	0/3/25/26	0/2/2/2
1	GF2	B	216	1	-	0/3/25/26	0/3/3/3
1	CFZ	C	301	1	-	0/2/22/26	0/2/2/2
1	GF2	C	302	1	-	0/3/25/26	0/3/3/3
1	AF2	C	303	1	-	0/3/25/26	0/3/3/3
1	AF2	C	304	1	-	0/3/25/26	0/3/3/3
1	UFT	C	305	1	-	0/3/25/26	0/2/2/2
1	UFT	C	306[A]	1	-	0/3/25/26	0/2/2/2
1	UFT	C	306[B]	1	-	0/3/25/26	0/2/2/2
1	CFZ	C	307[A]	1	-	0/3/25/26	0/2/2/2
1	CFZ	C	307[B]	1	-	0/3/25/26	0/2/2/2
1	GF2	C	308	1	-	0/3/25/26	0/3/3/3
1	CFZ	D	409[A]	1	-	0/2/22/26	0/2/2/2
1	CFZ	D	409[B]	1	-	0/2/22/26	0/2/2/2
1	GF2	D	410[A]	1	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GF2	D	410[B]	1	-	0/3/25/26	0/3/3/3
1	AF2	D	411[A]	1	-	0/3/25/26	0/3/3/3
1	AF2	D	411[B]	1	-	0/3/25/26	0/3/3/3
1	AF2	D	412	1	-	0/3/25/26	0/3/3/3
1	UFT	D	413[A]	1	-	0/3/25/26	0/2/2/2
1	UFT	D	413[B]	1	-	0/3/25/26	0/2/2/2
1	UFT	D	414[A]	1	-	0/3/25/26	0/2/2/2
1	UFT	D	414[B]	1	-	0/3/25/26	0/2/2/2
1	CFZ	D	415	1	-	0/3/25/26	0/2/2/2
1	GF2	D	416	1	-	0/3/25/26	0/3/3/3
1	CFZ	E	501	1	-	0/2/22/26	0/2/2/2
1	GF2	E	502	1	-	0/3/25/26	0/3/3/3
1	AF2	E	503	1	-	0/3/25/26	0/3/3/3
1	AF2	E	504	1	-	0/3/25/26	0/3/3/3
1	UFT	E	505	1,2	-	0/3/25/26	0/2/2/2
1	UFT	E	506	1	-	0/3/25/26	0/2/2/2
1	CFZ	E	507	1	-	0/3/25/26	0/2/2/2
1	GF2	E	508	1	-	0/3/25/26	0/3/3/3
1	CFZ	F	609	1	-	0/2/22/26	0/2/2/2
1	GF2	F	610	1	-	0/3/25/26	0/3/3/3
1	AF2	F	611	1	-	0/3/25/26	0/3/3/3
1	AF2	F	612	1	-	0/3/25/26	0/3/3/3
1	UFT	F	613	1	-	0/3/25/26	0/2/2/2
1	UFT	F	614	1	-	0/3/25/26	0/2/2/2
1	CFZ	F	615	1	-	0/3/25/26	0/2/2/2
1	GF2	F	616	1,2	-	0/3/25/26	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	414[A]	UFT	C6-C5	-2.96	1.31	1.38
1	D	414[B]	UFT	C6-C5	-2.96	1.31	1.38
1	F	614	UFT	C6-C5	-2.56	1.32	1.38
1	B	212	AF2	C8-N7	-2.54	1.29	1.34
1	B	216	GF2	C8-N7	-2.26	1.30	1.34
1	E	501	CFZ	C6-C5	-2.21	1.33	1.38
1	B	209	CFZ	C6-C5	-2.17	1.33	1.38
1	D	410[B]	GF2	C8-N7	-2.08	1.30	1.34
1	E	502	GF2	C2'-C1'	-2.03	1.50	1.53
1	C	306[A]	UFT	C6-C5	-2.02	1.33	1.38
1	A	104	AF2	C4-N3	-2.00	1.32	1.35
1	B	209	CFZ	O4'-C1'	2.02	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GF2	C2-N1	2.04	1.39	1.35
1	C	305	UFT	C6-N1	2.04	1.38	1.35
1	B	211	AF2	O4'-C1'	2.12	1.43	1.41
1	D	409[A]	CFZ	O4'-C1'	2.13	1.43	1.41
1	E	501	CFZ	O4'-C1'	2.15	1.43	1.41
1	D	413[A]	UFT	O4'-C1'	2.17	1.43	1.41
1	D	411[B]	AF2	C2-N3	2.24	1.36	1.32
1	D	411[A]	AF2	C2-N3	2.24	1.36	1.32
1	A	108	GF2	O4'-C1'	2.28	1.44	1.41
1	E	506	UFT	C4-N3	2.35	1.37	1.33
1	F	614	UFT	C4-N3	2.36	1.37	1.33
1	A	106	UFT	O4'-C1'	2.38	1.44	1.41
1	A	105	UFT	C4-N3	2.39	1.37	1.33
1	E	503	AF2	O4'-C1'	2.40	1.44	1.41
1	C	308	GF2	C6-N1	2.52	1.37	1.33
1	D	414[A]	UFT	C4-N3	2.54	1.37	1.33
1	D	414[B]	UFT	C4-N3	2.54	1.37	1.33
1	B	214	UFT	C4-N3	2.74	1.38	1.33
1	C	306[A]	UFT	C4-N3	2.79	1.38	1.33
1	C	306[B]	UFT	C4-N3	2.82	1.38	1.33
1	C	305	UFT	C4-N3	2.86	1.38	1.33
1	A	106	UFT	C4-N3	2.92	1.38	1.33
1	F	613	UFT	C4-N3	2.93	1.38	1.33
1	D	413[A]	UFT	C4-N3	2.97	1.38	1.33
1	D	413[B]	UFT	C4-N3	3.02	1.38	1.33
1	B	213	UFT	C4-N3	3.14	1.38	1.33
1	F	614	UFT	O4'-C1'	3.16	1.45	1.41
1	D	416	GF2	O4'-C1'	3.21	1.45	1.41
1	C	308	GF2	O4'-C1'	3.23	1.45	1.41
1	D	416	GF2	C6-N1	3.28	1.39	1.33
1	E	505	UFT	C4-N3	3.43	1.39	1.33
1	B	210	GF2	C6-N1	3.49	1.39	1.33
1	E	508	GF2	C6-N1	3.52	1.39	1.33
1	A	102	GF2	C6-N1	3.60	1.39	1.33
1	D	410[B]	GF2	C6-N1	3.64	1.39	1.33
1	B	216	GF2	C6-N1	3.67	1.39	1.33
1	C	302	GF2	C6-N1	3.77	1.40	1.33
1	D	410[A]	GF2	C6-N1	3.88	1.40	1.33
1	F	616	GF2	C6-N1	3.97	1.40	1.33
1	E	502	GF2	C6-N1	3.98	1.40	1.33
1	F	610	GF2	C6-N1	4.03	1.40	1.33
1	B	210	GF2	O4'-C1'	4.25	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GF2	C6-N1	4.72	1.41	1.33
1	E	502	GF2	O4'-C1'	4.95	1.47	1.41

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	508	GF2	C5-C6-N1	-8.98	111.31	123.59
1	B	210	GF2	C5-C6-N1	-8.59	111.85	123.59
1	D	416	GF2	C5-C6-N1	-8.52	111.94	123.59
1	D	410[B]	GF2	C5-C6-N1	-8.46	112.02	123.59
1	A	102	GF2	C5-C6-N1	-8.40	112.11	123.59
1	E	502	GF2	C5-C6-N1	-8.31	112.22	123.59
1	B	216	GF2	C5-C6-N1	-8.22	112.34	123.59
1	C	302	GF2	C5-C6-N1	-8.16	112.43	123.59
1	D	410[A]	GF2	C5-C6-N1	-8.11	112.50	123.59
1	C	308	GF2	C5-C6-N1	-8.10	112.52	123.59
1	F	610	GF2	C5-C6-N1	-7.54	113.28	123.59
1	F	616	GF2	C5-C6-N1	-7.49	113.35	123.59
1	A	108	GF2	C5-C6-N1	-7.32	113.58	123.59
1	F	612	AF2	N3-C2-N1	-4.76	125.25	128.89
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	A	104	AF2	N3-C2-N1	-4.07	125.78	128.89
1	D	414[A]	UFT	F2'-C2'-C1'	-3.80	100.35	109.54
1	D	414[B]	UFT	F2'-C2'-C1'	-3.80	100.35	109.54
1	C	302	GF2	N3-C2-N1	-3.59	121.97	127.44
1	B	213	UFT	C5-C4-N3	-3.41	114.37	123.12
1	F	614	UFT	C5-C4-N3	-3.40	114.39	123.12
1	F	611	AF2	C2'-C1'-N9	-3.36	107.77	113.76
1	C	306[B]	UFT	C5-C4-N3	-3.35	114.52	123.12
1	D	414[A]	UFT	C5-C4-N3	-3.31	114.63	123.12
1	D	414[B]	UFT	C5-C4-N3	-3.31	114.63	123.12
1	B	214	UFT	C5-C4-N3	-3.24	114.80	123.12
1	E	501	CFZ	F2'-C2'-C1'	-3.22	101.76	109.54
1	C	305	UFT	C5-C4-N3	-3.21	114.89	123.12
1	D	413[B]	UFT	C5-C4-N3	-3.17	114.99	123.12
1	D	413[A]	UFT	C5-C4-N3	-3.16	115.01	123.12
1	B	209	CFZ	F2'-C2'-C1'	-3.16	101.91	109.54
1	A	106	UFT	F2'-C2'-C1'	-3.14	101.95	109.54
1	E	505	UFT	C5-C4-N3	-3.12	115.13	123.12
1	C	308	GF2	N3-C2-N1	-3.02	122.85	127.44
1	A	105	UFT	C5-C4-N3	-3.01	115.39	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306[A]	UFT	C4'-O4'-C1'	-3.01	106.41	109.72
1	A	106	UFT	C5-C4-N3	-2.97	115.50	123.12
1	B	211	AF2	F-C2'-C1'	-2.96	102.37	109.54
1	F	613	UFT	C5-C4-N3	-2.92	115.62	123.12
1	E	508	GF2	C2'-C1'-N9	-2.77	108.81	113.76
1	E	502	GF2	F-C2'-C1'	-2.72	102.95	109.54
1	D	416	GF2	N3-C2-N1	-2.67	123.37	127.44
1	E	503	AF2	F-C2'-C1'	-2.63	103.17	109.54
1	B	211	AF2	N3-C2-N1	-2.62	126.89	128.89
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	C	306[A]	UFT	C5-C4-N3	-2.57	116.54	123.12
1	B	213	UFT	F2'-C2'-C1'	-2.55	103.38	109.54
1	E	506	UFT	C5-C4-N3	-2.54	116.60	123.12
1	B	211	AF2	C1'-N9-C4	-2.50	123.17	126.94
1	E	502	GF2	O4'-C1'-N9	-2.49	102.88	108.10
1	C	301	CFZ	F2'-C2'-C1'	-2.48	103.54	109.54
1	B	216	GF2	C2'-C1'-N9	-2.48	109.34	113.76
1	E	505	UFT	C6-N1-C2	-2.46	117.29	121.28
1	A	103	AF2	C2'-C1'-N9	-2.36	109.55	113.76
1	D	412	AF2	C2'-C1'-N9	-2.32	109.62	113.76
1	B	210	GF2	O4'-C1'-N9	-2.29	103.31	108.10
1	C	302	GF2	C6-C5-C4	-2.27	118.19	120.90
1	F	614	UFT	F2'-C2'-C1'	-2.25	104.09	109.54
1	E	506	UFT	F2'-C2'-C1'	-2.22	104.18	109.54
1	A	102	GF2	C2'-C1'-N9	-2.22	109.80	113.76
1	D	416	GF2	F-C2'-C1'	-2.21	104.20	109.54
1	B	210	GF2	F-C2'-C1'	-2.20	104.21	109.54
1	C	307[A]	CFZ	F2'-C2'-C1'	-2.20	104.22	109.54
1	C	307[B]	CFZ	F2'-C2'-C1'	-2.20	104.22	109.54
1	B	214	UFT	F2'-C2'-C1'	-2.17	104.29	109.54
1	F	610	GF2	C6-C5-C4	-2.13	118.35	120.90
1	D	410[B]	GF2	N3-C2-N1	-2.13	124.21	127.44
1	D	414[A]	UFT	F2'-C2'-C3'	-2.11	103.95	109.07
1	D	414[B]	UFT	F2'-C2'-C3'	-2.11	103.95	109.07
1	B	213	UFT	C6-N1-C2	-2.10	117.88	121.28
1	D	412	AF2	C1'-N9-C4	-2.10	123.78	126.94
1	A	107	CFZ	N4-C4-N3	2.05	120.24	116.50
1	B	210	GF2	C4-C5-N7	2.07	111.38	109.48
1	B	209	CFZ	O4'-C1'-C2'	2.08	108.19	105.84
1	C	304	AF2	N3-C2-N1	2.09	130.49	128.89
1	C	304	AF2	O4'-C1'-C2'	2.10	108.22	105.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306[A]	UFT	O3'-C3'-C2'	2.18	119.25	111.68
1	B	210	GF2	O4'-C1'-C2'	2.19	108.32	105.84
1	E	503	AF2	O4'-C1'-C2'	2.19	108.32	105.84
1	F	611	AF2	O4'-C1'-C2'	2.23	108.37	105.84
1	D	409[B]	CFZ	O4'-C1'-C2'	2.23	108.37	105.84
1	D	412	AF2	N6-C6-N1	2.23	123.99	119.20
1	B	215	CFZ	O4'-C1'-C2'	2.24	108.39	105.84
1	C	304	AF2	C4-C5-N7	2.39	111.68	109.48
1	B	213	UFT	C6-C5-C4	2.57	122.09	117.28
1	C	305	UFT	O4'-C1'-C2'	2.59	108.78	105.84
1	B	214	UFT	C6-C5-C4	2.59	122.13	117.28
1	A	104	AF2	C4-C5-N7	2.63	111.89	109.48
1	B	211	AF2	O4'-C1'-C2'	2.63	108.83	105.84
1	E	501	CFZ	C2-N3-C4	2.64	119.34	115.61
1	D	413[A]	UFT	O4'-C1'-C2'	2.78	108.99	105.84
1	C	306[A]	UFT	O4'-C1'-C2'	2.79	109.01	105.84
1	A	101	CFZ	C2-N3-C4	2.84	119.62	115.61
1	E	502	GF2	C4-C5-N7	2.86	112.11	109.48
1	D	412	AF2	O4'-C1'-C2'	2.95	109.19	105.84
1	B	210	GF2	C2'-C1'-N9	2.99	119.10	113.76
1	F	609	CFZ	C2-N3-C4	3.00	119.84	115.61
1	D	409[B]	CFZ	C2-N3-C4	3.04	119.90	115.61
1	E	502	GF2	C2'-C1'-N9	3.09	119.28	113.76
1	D	412	AF2	C4-C5-N7	3.17	112.40	109.48
1	E	501	CFZ	O4'-C1'-C2'	3.19	109.46	105.84
1	E	502	GF2	O4'-C1'-C2'	3.30	109.59	105.84
1	D	409[A]	CFZ	C2-N3-C4	3.60	120.69	115.61
1	A	107	CFZ	C2-N3-C4	3.72	120.86	115.61
1	E	507	CFZ	C2-N3-C4	3.74	120.89	115.61
1	A	108	GF2	C6-N1-C2	3.80	121.21	115.94
1	C	307[A]	CFZ	C2-N3-C4	3.81	120.99	115.61
1	C	307[B]	CFZ	C2-N3-C4	3.81	120.99	115.61
1	F	615	CFZ	C2-N3-C4	4.15	121.46	115.61
1	D	415	CFZ	C2-N3-C4	4.18	121.50	115.61
1	B	215	CFZ	C2-N3-C4	4.24	121.59	115.61
1	F	616	GF2	C6-N1-C2	4.44	122.11	115.94
1	C	301	CFZ	C2-N3-C4	4.54	122.01	115.61
1	F	610	GF2	C6-N1-C2	4.88	122.72	115.94
1	E	508	GF2	C6-N1-C2	5.35	123.37	115.94
1	D	410[A]	GF2	C6-N1-C2	5.37	123.39	115.94
1	B	216	GF2	C6-N1-C2	5.39	123.42	115.94
1	A	102	GF2	C6-N1-C2	5.39	123.42	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	GF2	C6-N1-C2	5.44	123.49	115.94
1	E	502	GF2	C6-N1-C2	5.62	123.75	115.94
1	D	410[B]	GF2	C6-N1-C2	5.94	124.18	115.94
1	C	308	GF2	C6-N1-C2	6.32	124.72	115.94
1	D	416	GF2	C6-N1-C2	6.57	125.06	115.94
1	C	302	GF2	C6-N1-C2	6.98	125.63	115.94
1	B	213	UFT	C4-N3-C2	9.34	123.39	114.14
1	E	505	UFT	C4-N3-C2	10.16	124.21	114.14
1	C	306[A]	UFT	C4-N3-C2	11.28	125.31	114.14
1	B	214	UFT	C4-N3-C2	11.32	125.35	114.14
1	E	506	UFT	C4-N3-C2	11.75	125.77	114.14
1	A	106	UFT	C4-N3-C2	12.46	126.48	114.14
1	C	306[B]	UFT	C4-N3-C2	12.67	126.69	114.14
1	F	614	UFT	C4-N3-C2	12.77	126.79	114.14
1	D	414[A]	UFT	C4-N3-C2	12.88	126.90	114.14
1	D	414[B]	UFT	C4-N3-C2	12.88	126.90	114.14
1	F	613	UFT	C4-N3-C2	13.06	127.07	114.14
1	A	105	UFT	C4-N3-C2	13.29	127.30	114.14
1	D	413[B]	UFT	C4-N3-C2	13.32	127.33	114.14
1	D	413[A]	UFT	C4-N3-C2	14.45	128.45	114.14
1	C	305	UFT	C4-N3-C2	15.00	128.99	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	104	AF2	1	0
1	A	105	UFT	1	0
1	B	209	CFZ	1	0
1	B	210	GF2	1	0
1	B	213	UFT	2	0
1	B	214	UFT	2	0
1	C	301	CFZ	1	0
1	C	302	GF2	1	0
1	C	306[B]	UFT	1	0
1	D	409[A]	CFZ	1	0
1	D	409[B]	CFZ	2	0
1	D	410[A]	GF2	1	0
1	D	410[B]	GF2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	415	CFZ	1	0
1	E	501	CFZ	1	0
1	E	502	GF2	1	0
1	E	505	UFT	1	0
1	E	506	UFT	1	0
1	F	612	AF2	1	0
1	F	613	UFT	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	0/8	-	-	-	-
1	B	0/8	-	-	-	-
1	C	0/8	-	-	-	-
1	D	0/8	-	-	-	-
1	E	0/8	-	-	-	-
1	F	0/8	-	-	-	-
All	All	0/48	-	-	-	-

There are no RSRZ outliers to report.

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GF2	F	616	23/24	0.99	0.05	-	8,9,13,15	0
1	GF2	D	410[A]	23/24	0.99	0.07	-	8,9,9,10	23
1	UFT	F	614	20/21	0.98	0.06	-	11,12,18,18	0
1	AF2	E	504	22/23	0.98	0.06	-	10,13,17,20	0
1	GF2	D	410[B]	23/24	0.99	0.07	-	7,9,14,16	23
1	AF2	C	303	22/23	0.98	0.06	-	9,10,12,15	0
1	GF2	F	610	23/24	0.96	0.07	-	12,15,24,31	0
1	CFZ	F	615	20/21	0.99	0.06	-	9,11,14,17	0
1	GF2	B	216	23/24	0.97	0.07	-	15,17,20,22	0
1	CFZ	D	415	20/21	0.96	0.08	-	10,15,27,31	0
1	UFT	C	306[A]	20/21	0.94	0.11	-	16,20,28,29	20
1	UFT	B	213	20/21	0.97	0.06	-	13,16,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	AF2	D	412	22/23	0.98	0.07	-	11,15,22,23	0
1	UFT	C	306[B]	20/21	0.94	0.11	-	16,21,30,31	20
1	UFT	E	505	20/21	0.97	0.08	-	14,16,19,19	0
1	CFZ	A	107	20/21	0.99	0.06	-	9,12,15,17	0
1	UFT	A	106	20/21	0.98	0.06	-	10,12,18,19	0
1	UFT	F	613	20/21	0.98	0.07	-	9,11,20,21	0
1	UFT	B	214	20/21	0.97	0.08	-	13,15,21,23	0
1	AF2	F	611	22/23	0.97	0.07	-	12,14,18,22	0
1	CFZ	C	307[A]	20/21	0.95	0.09	-	10,15,26,26	5
1	CFZ	B	209	17/21	0.98	0.06	-	10,12,16,19	0
1	CFZ	F	609	17/21	0.95	0.07	-	19,22,27,35	0
1	UFT	E	506	20/21	0.97	0.07	-	13,14,23,24	0
1	UFT	D	414[A]	20/21	0.93	0.10	-	17,22,27,29	0
1	CFZ	C	307[B]	20/21	0.95	0.09	-	10,15,27,30	5
1	CFZ	E	501	17/21	0.97	0.07	-	10,12,15,19	0
1	UFT	A	105	20/21	0.98	0.07	-	10,11,20,21	0
1	CFZ	D	409[B]	17/21	0.98	0.07	-	8,11,18,18	17
1	GF2	A	108	23/24	0.99	0.05	-	8,9,12,14	0
1	UFT	D	414[B]	20/21	0.93	0.10	-	17,22,26,35	5
1	CFZ	D	409[A]	17/21	0.98	0.07	-	9,10,12,13	17
1	AF2	D	411[B]	22/23	0.99	0.06	-	8,10,15,15	5
1	CFZ	C	301	17/21	0.98	0.06	-	9,10,13,15	0
1	GF2	E	502	23/24	0.98	0.06	-	9,11,14,16	0
1	GF2	A	102	23/24	0.96	0.07	-	13,15,24,27	0
1	AF2	D	411[A]	22/23	0.99	0.06	-	8,10,11,12	5
1	UFT	C	305	20/21	0.98	0.07	-	12,18,27,27	0
1	AF2	E	503	22/23	0.97	0.07	-	11,12,14,16	0
1	GF2	C	308	23/24	0.98	0.06	-	8,11,18,21	0
1	CFZ	A	101	17/21	0.96	0.07	-	19,23,33,51	0
1	CFZ	B	215	20/21	0.98	0.06	-	12,14,16,17	0
1	GF2	D	416	23/24	0.97	0.07	-	9,11,17,22	0
1	AF2	B	211	22/23	0.98	0.06	-	10,12,14,16	0
1	GF2	C	302	23/24	0.98	0.06	-	8,9,11,11	0
1	UFT	D	413[B]	20/21	0.98	0.09	-	13,20,28,29	20
1	GF2	B	210	23/24	0.98	0.07	-	9,12,14,16	0
1	GF2	E	508	23/24	0.98	0.07	-	16,17,21,24	0
1	UFT	D	413[A]	20/21	0.98	0.09	-	11,18,25,25	20
1	AF2	A	104	22/23	0.96	0.08	-	11,13,17,21	0
1	AF2	A	103	22/23	0.97	0.06	-	12,15,18,23	0
1	AF2	B	212	22/23	0.98	0.06	-	10,13,17,18	0
1	CFZ	E	507	20/21	0.98	0.06	-	11,14,16,16	0
1	AF2	C	304	22/23	0.98	0.07	-	11,16,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	AF2	F	612	22/23	0.96	0.08	-	11,14,17,22	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SR	E	703	1/1	1.00	0.15	-	18,18,18,18	1
2	SR	D	702	1/1	0.99	0.22	-	20,20,20,20	0
2	SR	F	706	1/1	0.99	0.28	-	18,18,18,18	1
2	SR	D	708	1/1	1.00	0.22	-	23,23,23,23	0
3	MG	E	712	1/1	0.99	0.25	-	21,21,21,21	1
2	SR	C	701	1/1	0.99	0.24	-	21,21,21,21	0
2	SR	A	705	1/1	0.99	0.23	-	32,32,32,32	0
2	SR	E	709	1/1	0.97	0.14	-	28,28,28,28	1
2	SR	B	704	1/1	1.00	0.14	-	18,18,18,18	1
3	MG	B	711	1/1	0.99	0.23	-	19,19,19,19	1
2	SR	C	707	1/1	1.00	0.23	-	23,23,23,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.