



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:26 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

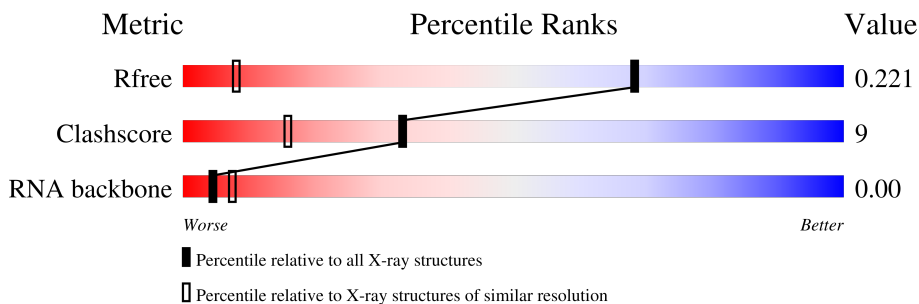
1 Overall quality at a glance

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}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
RNA backbone	3102	1000 (2.34-0.62)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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
			Total	C	F	N	O	P			
1	A	8	Total 167	C 76	F 8	N 30	O 46	P 7	0	0	0
1	B	8	Total 167	C 76	F 8	N 30	O 46	P 7	0	0	0
1	C	8	Total 192	C 86	F 9	N 32	O 56	P 9	0	2	0
1	D	8	Total 237	C 106	F 11	N 40	O 69	P 11	0	5	0
1	E	8	Total 167	C 76	F 8	N 30	O 46	P 7	0	0	0
1	F	8	Total 167	C 76	F 8	N 30	O 46	P 7	0	0	0

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

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

- 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

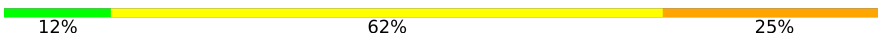
- Molecule 4 is water.

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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 

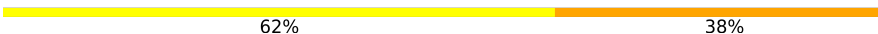


- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain B: 

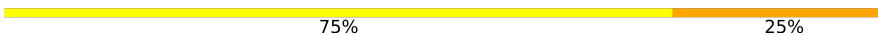


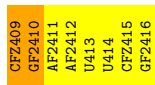
- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain C: 



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

Chain D: 

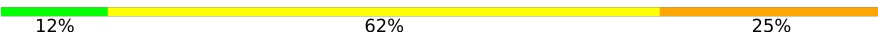


- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain E: 



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

Chain F: 

CFZ609
GF2610
AF2611
AF2612
U613
U614
CFZ615
GF2616

4 Data and refinement statistics i

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	2.60 (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	1998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.487 for h,-h-k,-l 0.028 for -k,-h,-l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SR, AF2, MG, GF2, UFT, CFZ

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 [i](#)

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	UFT	D	413[B]	1	18,21,22	0.30	0	26,30,33	0.82	2 (7%)
1	CFZ	F	615	1	18,21,22	0.39	0	26,30,33	0.96	1 (3%)
1	GF2	E	508	1	18,25,26	1.14	2 (11%)	19,37,40	1.29	3 (15%)
1	UFT	E	506	1	18,21,22	0.46	0	26,30,33	1.26	3 (11%)
1	UFT	C	306[B]	1	18,21,22	0.47	0	26,30,33	0.62	0
1	GF2	E	502	1	18,25,26	1.63	5 (27%)	19,37,40	1.52	3 (15%)
1	CFZ	A	101	1	18,18,22	0.38	0	26,26,33	0.85	0
1	AF2	B	211	1	18,24,25	0.85	1 (5%)	18,35,38	1.66	4 (22%)
1	CFZ	A	107	1	18,21,22	0.47	0	26,30,33	0.97	1 (3%)
1	CFZ	B	215	1	18,21,22	0.55	0	26,30,33	1.19	3 (11%)
1	UFT	E	505	1,2	18,21,22	0.59	0	26,30,33	1.65	4 (15%)
1	AF2	A	104	1	18,24,25	0.91	1 (5%)	18,35,38	1.30	2 (11%)
1	AF2	F	611	1	18,24,25	0.80	0	18,35,38	1.23	3 (16%)
1	UFT	F	614	1	18,21,22	0.72	0	26,30,33	1.21	3 (11%)
1	AF2	C	304	1	18,24,25	0.81	0	18,35,38	1.35	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	F	609	1	18,18,22	0.38	0	26,26,33	0.72	0
1	AF2	A	103	1	18,24,25	0.74	1 (5%)	18,35,38	1.37	2 (11%)
1	GF2	F	610	1	18,25,26	1.13	2 (11%)	19,37,40	1.01	1 (5%)
1	GF2	A	102	1	18,25,26	1.10	2 (11%)	19,37,40	1.12	2 (10%)
1	CFZ	E	501	1	18,18,22	0.57	0	26,26,33	1.23	3 (11%)
1	AF2	D	411[A]	1	18,24,25	0.83	1 (5%)	18,35,38	1.18	1 (5%)
1	CFZ	C	301	1	18,18,22	0.60	0	26,26,33	1.02	2 (7%)
1	GF2	D	416	1	18,25,26	1.32	4 (22%)	19,37,40	1.06	2 (10%)
1	AF2	E	503	1	18,24,25	0.86	1 (5%)	18,35,38	1.42	5 (27%)
1	UFT	B	213	1,2	18,21,22	0.65	0	26,30,33	1.64	7 (26%)
1	AF2	D	411[B]	1	18,24,25	0.84	1 (5%)	18,35,38	1.20	1 (5%)
1	CFZ	B	209	1	18,18,22	0.60	0	26,26,33	1.21	3 (11%)
1	CFZ	D	409[A]	1	18,18,22	0.57	0	26,26,33	1.10	2 (7%)
1	CFZ	E	507	1	18,21,22	0.44	0	26,30,33	1.02	1 (3%)
1	AF2	D	412	1	18,24,25	0.79	0	18,35,38	1.60	4 (22%)
1	CFZ	D	409[B]	1	18,18,22	0.37	0	26,26,33	0.81	2 (7%)
1	UFT	F	613	1	18,21,22	0.57	0	26,30,33	1.04	2 (7%)
1	GF2	D	410[A]	1	18,25,26	1.25	3 (16%)	19,37,40	1.36	3 (15%)
1	AF2	C	303	1	18,24,25	0.82	0	18,35,38	1.01	1 (5%)
1	AF2	F	612	1	18,24,25	0.92	0	18,35,38	1.34	3 (16%)
1	GF2	F	616	1,2	18,25,26	1.10	2 (11%)	19,37,40	1.02	0
1	UFT	A	106	1	18,21,22	0.62	0	26,30,33	1.21	2 (7%)
1	GF2	D	410[B]	1	18,25,26	1.12	3 (16%)	19,37,40	1.09	2 (10%)
1	UFT	A	105	1	18,21,22	0.70	0	26,30,33	0.87	1 (3%)
1	GF2	C	308	1	18,25,26	1.28	3 (16%)	19,37,40	0.94	1 (5%)
1	UFT	B	214	1	18,21,22	0.36	0	26,30,33	1.18	3 (11%)
1	CFZ	C	307[A]	1	18,21,22	0.54	0	26,30,33	0.98	1 (3%)
1	AF2	E	504	1	18,24,25	0.83	0	18,35,38	1.39	3 (16%)
1	UFT	D	414[A]	1	18,21,22	0.70	0	26,30,33	1.70	5 (19%)
1	AF2	B	212	1	18,24,25	0.91	1 (5%)	18,35,38	1.50	4 (22%)
1	GF2	C	302	1	18,25,26	1.19	2 (11%)	19,37,40	1.10	2 (10%)
1	CFZ	C	307[B]	1	18,21,22	0.51	0	26,30,33	1.01	1 (3%)
1	UFT	D	413[A]	1	18,21,22	0.44	0	26,30,33	1.19	3 (11%)
1	UFT	D	414[B]	1	18,21,22	0.68	0	26,30,33	1.69	5 (19%)
1	GF2	B	216	1	18,25,26	1.18	3 (16%)	19,37,40	1.60	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GF2	A	108	1,2	18,25,26	1.39	5 (27%)	19,37,40	1.16	3 (15%)
1	CFZ	D	415	1	18,21,22	0.58	0	26,30,33	1.01	0
1	UFT	C	305	1	18,21,22	0.49	0	26,30,33	1.34	3 (11%)
1	UFT	C	306[A]	1	18,21,22	0.60	0	26,30,33	1.39	3 (11%)
1	GF2	B	210	1	18,25,26	1.51	4 (22%)	19,37,40	1.37	4 (21%)

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	UFT	D	413[B]	1	-	0/7/25/26	0/2/2/2
1	CFZ	F	615	1	-	0/7/25/26	0/2/2/2
1	GF2	E	508	1	-	0/3/25/26	0/3/3/3
1	UFT	E	506	1	-	0/7/25/26	0/2/2/2
1	UFT	C	306[B]	1	-	2/7/25/26	0/2/2/2
1	GF2	E	502	1	-	0/3/25/26	0/3/3/3
1	CFZ	A	101	1	-	0/6/22/26	0/2/2/2
1	AF2	B	211	1	-	0/3/25/26	0/3/3/3
1	CFZ	A	107	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	215	1	-	0/7/25/26	0/2/2/2
1	UFT	E	505	1,2	-	0/7/25/26	0/2/2/2
1	AF2	A	104	1	-	0/3/25/26	0/3/3/3
1	AF2	F	611	1	-	0/3/25/26	0/3/3/3
1	UFT	F	614	1	-	0/7/25/26	0/2/2/2
1	AF2	C	304	1	-	0/3/25/26	0/3/3/3
1	CFZ	F	609	1	-	1/6/22/26	0/2/2/2
1	AF2	A	103	1	-	0/3/25/26	0/3/3/3
1	GF2	F	610	1	-	0/3/25/26	0/3/3/3
1	GF2	A	102	1	-	0/3/25/26	0/3/3/3
1	CFZ	E	501	1	-	0/6/22/26	0/2/2/2
1	AF2	D	411[A]	1	-	0/3/25/26	0/3/3/3
1	CFZ	C	301	1	-	0/6/22/26	0/2/2/2
1	GF2	D	416	1	-	0/3/25/26	0/3/3/3
1	AF2	E	503	1	-	0/3/25/26	0/3/3/3
1	UFT	B	213	1,2	-	0/7/25/26	0/2/2/2
1	AF2	D	411[B]	1	-	0/3/25/26	0/3/3/3
1	CFZ	B	209	1	-	0/6/22/26	0/2/2/2
1	CFZ	D	409[A]	1	-	0/6/22/26	0/2/2/2
1	CFZ	E	507	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AF2	D	412	1	-	0/3/25/26	0/3/3/3
1	CFZ	D	409[B]	1	-	0/6/22/26	0/2/2/2
1	UFT	F	613	1	-	0/7/25/26	0/2/2/2
1	GF2	D	410[A]	1	-	0/3/25/26	0/3/3/3
1	AF2	C	303	1	-	0/3/25/26	0/3/3/3
1	AF2	F	612	1	-	0/3/25/26	0/3/3/3
1	GF2	F	616	1,2	-	0/3/25/26	0/3/3/3
1	UFT	A	106	1	-	0/7/25/26	0/2/2/2
1	GF2	D	410[B]	1	-	0/3/25/26	0/3/3/3
1	UFT	A	105	1	-	0/7/25/26	0/2/2/2
1	GF2	C	308	1	-	0/3/25/26	0/3/3/3
1	UFT	B	214	1	-	0/7/25/26	0/2/2/2
1	CFZ	C	307[A]	1	-	0/7/25/26	0/2/2/2
1	AF2	E	504	1	-	0/3/25/26	0/3/3/3
1	UFT	D	414[A]	1	-	0/7/25/26	0/2/2/2
1	AF2	B	212	1	-	0/3/25/26	0/3/3/3
1	GF2	C	302	1	-	0/3/25/26	0/3/3/3
1	CFZ	C	307[B]	1	-	0/7/25/26	0/2/2/2
1	UFT	D	413[A]	1	-	0/7/25/26	0/2/2/2
1	UFT	D	414[B]	1	-	0/7/25/26	0/2/2/2
1	GF2	B	216	1	-	0/3/25/26	0/3/3/3
1	GF2	A	108	1,2	-	0/3/25/26	0/3/3/3
1	CFZ	D	415	1	-	0/7/25/26	0/2/2/2
1	UFT	C	305	1	-	0/7/25/26	0/2/2/2
1	UFT	C	306[A]	1	-	1/7/25/26	0/2/2/2
1	GF2	B	210	1	-	0/3/25/26	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	502	GF2	O4'-C1'	4.57	1.47	1.41
1	B	210	GF2	O4'-C1'	3.94	1.46	1.41
1	C	308	GF2	C5-C6	-3.11	1.41	1.47
1	C	308	GF2	O4'-C1'	3.01	1.45	1.41
1	D	416	GF2	O4'-C1'	3.00	1.45	1.41
1	C	302	GF2	C5-C6	-2.82	1.41	1.47
1	B	210	GF2	C5-C6	-2.80	1.41	1.47
1	B	216	GF2	C8-N7	-2.78	1.30	1.35
1	B	212	AF2	C8-N7	-2.78	1.29	1.34
1	C	302	GF2	C5-C4	-2.77	1.36	1.43
1	F	616	GF2	C5-C4	-2.70	1.36	1.43
1	A	108	GF2	C5-C4	-2.69	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GF2	C6-N1	2.68	1.41	1.37
1	D	416	GF2	C5-C6	-2.68	1.42	1.47
1	D	410[A]	GF2	C5-C6	-2.58	1.42	1.47
1	D	410[B]	GF2	C8-N7	-2.58	1.30	1.35
1	A	102	GF2	C5-C6	-2.54	1.42	1.47
1	D	411[A]	AF2	C2-N3	2.52	1.36	1.32
1	D	411[B]	AF2	C2-N3	2.52	1.36	1.32
1	F	610	GF2	C5-C6	-2.51	1.42	1.47
1	D	410[B]	GF2	C5-C6	-2.50	1.42	1.47
1	B	216	GF2	C5-C6	-2.47	1.42	1.47
1	A	102	GF2	C8-N7	-2.46	1.30	1.35
1	D	410[A]	GF2	C5-C4	-2.46	1.36	1.43
1	F	610	GF2	C8-N7	-2.43	1.30	1.35
1	C	308	GF2	C5-C4	-2.41	1.36	1.43
1	E	508	GF2	C5-C6	-2.40	1.42	1.47
1	D	410[A]	GF2	C8-N7	-2.38	1.31	1.35
1	E	502	GF2	C5-C6	-2.38	1.42	1.47
1	E	502	GF2	C8-N7	-2.34	1.31	1.35
1	E	508	GF2	C8-N7	-2.34	1.31	1.35
1	E	502	GF2	C2'-C1'	-2.33	1.50	1.53
1	A	108	GF2	C5-C6	-2.31	1.42	1.47
1	D	416	GF2	C5-C4	-2.30	1.37	1.43
1	A	108	GF2	C8-N7	-2.28	1.31	1.35
1	E	503	AF2	O4'-C1'	2.26	1.44	1.41
1	B	210	GF2	C5-C4	-2.26	1.37	1.43
1	A	104	AF2	C4-N3	-2.22	1.32	1.35
1	E	502	GF2	C5-C4	-2.18	1.37	1.43
1	B	210	GF2	C2'-C1'	-2.17	1.50	1.53
1	F	616	GF2	C5-C6	-2.16	1.43	1.47
1	A	108	GF2	O4'-C1'	2.16	1.44	1.41
1	D	416	GF2	C8-N7	-2.09	1.31	1.35
1	A	103	AF2	F-C2'	-2.03	1.35	1.40
1	B	216	GF2	C5-C4	-2.02	1.37	1.43
1	B	211	AF2	O4'-C1'	2.01	1.43	1.41
1	D	410[B]	GF2	C5-C4	-2.01	1.38	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	505	UFT	O2-C2-N1	-4.50	116.81	122.79
1	D	414[A]	UFT	F2'-C2'-C1'	-4.19	100.35	109.08
1	D	414[B]	UFT	F2'-C2'-C1'	-4.19	100.35	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	AF2	C5-C6-N6	4.19	126.71	120.35
1	E	502	GF2	O4'-C1'-C2'	3.69	109.59	105.79
1	B	213	UFT	N3-C2-N1	3.58	119.64	114.89
1	E	501	CFZ	O4'-C1'-C2'	3.56	109.46	105.79
1	B	216	GF2	O6-C6-N1	-3.53	116.48	120.65
1	E	501	CFZ	F2'-C2'-C1'	-3.51	101.76	109.08
1	B	216	GF2	O6-C6-C5	3.48	131.17	124.37
1	B	209	CFZ	F2'-C2'-C1'	-3.44	101.91	109.08
1	E	502	GF2	C3'-C2'-C1'	-3.42	98.98	103.13
1	A	106	UFT	F2'-C2'-C1'	-3.42	101.95	109.08
1	D	414[A]	UFT	C2'-C3'-C4'	-3.38	98.03	102.40
1	D	414[B]	UFT	C2'-C3'-C4'	-3.38	98.03	102.40
1	D	410[A]	GF2	C3'-C2'-C1'	-3.34	99.08	103.13
1	A	103	AF2	C5-C6-N6	3.33	125.41	120.35
1	D	412	AF2	O4'-C1'-C2'	3.30	109.19	105.79
1	E	507	CFZ	C3'-C2'-C1'	-3.23	99.22	103.13
1	B	211	AF2	F-C2'-C1'	-3.22	102.37	109.08
1	B	215	CFZ	C3'-C2'-C1'	-3.15	99.31	103.13
1	C	306[A]	UFT	O4'-C1'-C2'	3.12	109.01	105.79
1	D	413[A]	UFT	O4'-C1'-C2'	3.11	108.99	105.79
1	E	504	AF2	C3'-C2'-C1'	-3.02	99.48	103.13
1	F	611	AF2	C3'-C2'-C1'	-2.99	99.51	103.13
1	E	505	UFT	N3-C2-N1	2.96	118.82	114.89
1	B	211	AF2	O4'-C1'-C2'	2.95	108.83	105.79
1	E	502	GF2	F-C2'-C1'	-2.94	102.95	109.08
1	D	411[A]	AF2	C3'-C2'-C1'	-2.92	99.59	103.13
1	D	411[B]	AF2	C3'-C2'-C1'	-2.92	99.59	103.13
1	B	212	AF2	C3'-C2'-C1'	-2.92	99.60	103.13
1	A	103	AF2	C3'-C2'-C1'	-2.90	99.61	103.13
1	C	305	UFT	O4'-C1'-C2'	2.90	108.78	105.79
1	E	505	UFT	C6-N1-C2	-2.89	117.29	120.99
1	E	504	AF2	C5-C6-N6	2.89	124.75	120.35
1	E	508	GF2	C3'-C2'-C1'	-2.89	99.63	103.13
1	D	412	AF2	C4-C5-N7	2.88	112.40	109.40
1	D	412	AF2	C3'-C2'-C1'	-2.86	99.67	103.13
1	E	503	AF2	F-C2'-C1'	-2.83	103.17	109.08
1	B	216	GF2	C3'-C2'-C1'	-2.80	99.74	103.13
1	F	613	UFT	C3'-C2'-C1'	-2.80	99.74	103.13
1	B	209	CFZ	C3'-C2'-C1'	-2.78	99.76	103.13
1	D	409[A]	CFZ	C3'-C2'-C1'	-2.77	99.78	103.13
1	B	211	AF2	C3'-C2'-C1'	-2.75	99.80	103.13
1	B	213	UFT	F2'-C2'-C1'	-2.73	103.38	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	GF2	C3'-C2'-C1'	-2.73	99.83	103.13
1	D	410[A]	GF2	O6-C6-C5	2.70	129.66	124.37
1	E	508	GF2	O6-C6-C5	2.69	129.62	124.37
1	C	301	CFZ	F2'-C2'-C1'	-2.66	103.54	109.08
1	B	213	UFT	O2-C2-N1	-2.63	119.28	122.79
1	C	303	AF2	C3'-C2'-C1'	-2.63	99.95	103.13
1	C	301	CFZ	C3'-C2'-C1'	-2.63	99.95	103.13
1	F	614	UFT	C3'-C2'-C1'	-2.62	99.95	103.13
1	D	412	AF2	N6-C6-N1	2.61	123.99	118.57
1	C	302	GF2	C3'-C2'-C1'	-2.59	100.00	103.13
1	B	210	GF2	O6-C6-C5	2.58	129.41	124.37
1	B	211	AF2	C5-C6-N6	2.58	124.27	120.35
1	E	506	UFT	O4-C4-N3	-2.54	115.58	119.31
1	C	304	AF2	C3'-C2'-C1'	-2.52	100.08	103.13
1	D	414[A]	UFT	F2'-C2'-C3'	-2.52	103.95	109.22
1	D	414[B]	UFT	F2'-C2'-C3'	-2.52	103.95	109.22
1	B	215	CFZ	O4'-C1'-C2'	2.52	108.39	105.79
1	E	501	CFZ	C3'-C2'-C1'	-2.51	100.09	103.13
1	D	409[B]	CFZ	O4'-C1'-C2'	2.50	108.37	105.79
1	F	611	AF2	O4'-C1'-C2'	2.50	108.37	105.79
1	D	410[B]	GF2	C3'-C2'-C1'	-2.49	100.11	103.13
1	F	610	GF2	C3'-C2'-C1'	-2.46	100.15	103.13
1	E	503	AF2	O4'-C1'-C2'	2.46	108.32	105.79
1	B	210	GF2	O4'-C1'-C2'	2.45	108.32	105.79
1	B	213	UFT	C6-N1-C2	-2.43	117.88	120.99
1	B	213	UFT	C4-N3-C2	-2.42	123.39	126.58
1	A	107	CFZ	C3'-C2'-C1'	-2.41	100.21	103.13
1	A	106	UFT	C3'-C2'-C1'	-2.40	100.22	103.13
1	A	104	AF2	C4-C5-N7	2.39	111.89	109.40
1	F	614	UFT	F2'-C2'-C1'	-2.39	104.09	109.08
1	D	410[B]	GF2	O6-C6-C5	2.38	129.03	124.37
1	F	615	CFZ	C3'-C2'-C1'	-2.38	100.25	103.13
1	F	611	AF2	C5-C6-N6	2.38	123.96	120.35
1	D	410[A]	GF2	O6-C6-N1	-2.38	117.84	120.65
1	B	215	CFZ	C2'-C1'-N1	-2.37	110.58	114.20
1	F	614	UFT	O4-C4-N3	2.37	122.78	119.31
1	C	304	AF2	O4'-C1'-C2'	2.36	108.22	105.79
1	E	506	UFT	F2'-C2'-C1'	-2.35	104.18	109.08
1	B	213	UFT	C1'-N1-C6	2.35	125.97	120.84
1	D	416	GF2	F-C2'-C1'	-2.34	104.20	109.08
1	F	612	AF2	C5-C6-N6	2.34	123.91	120.35
1	E	503	AF2	C5-C6-N6	2.34	123.90	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	GF2	F-C2'-C1'	-2.34	104.21	109.08
1	B	209	CFZ	O4'-C1'-C2'	2.33	108.19	105.79
1	C	307[A]	CFZ	F2'-C2'-C1'	-2.33	104.22	109.08
1	C	307[B]	CFZ	F2'-C2'-C1'	-2.33	104.22	109.08
1	B	214	UFT	F2'-C2'-C1'	-2.30	104.29	109.08
1	B	216	GF2	C8-N7-C5	2.30	107.37	102.99
1	B	214	UFT	C3'-C2'-C1'	-2.28	100.36	103.13
1	E	504	AF2	C5-C6-N1	-2.26	115.22	120.35
1	A	108	GF2	O6-C6-N1	-2.24	118.00	120.65
1	F	612	AF2	O4'-C1'-C2'	2.24	108.10	105.79
1	E	505	UFT	C1'-N1-C6	2.23	125.71	120.84
1	A	102	GF2	C3'-C2'-C1'	-2.21	100.45	103.13
1	D	416	GF2	O6-C6-C5	2.21	128.69	124.37
1	D	413[B]	UFT	F2'-C2'-C3'	-2.21	104.59	109.22
1	D	414[A]	UFT	O2-C2-N3	2.21	125.61	121.50
1	D	414[B]	UFT	O2-C2-N3	2.21	125.61	121.50
1	D	409[A]	CFZ	O2-C2-N1	-2.21	114.34	118.89
1	F	612	AF2	N3-C2-N1	-2.20	125.25	128.68
1	D	413[A]	UFT	O2-C2-N3	2.19	125.59	121.50
1	E	503	AF2	C3'-C2'-C1'	-2.19	100.47	103.13
1	D	413[B]	UFT	O4'-C1'-C2'	2.19	108.05	105.79
1	C	304	AF2	C4-C5-N7	2.18	111.68	109.40
1	B	212	AF2	O4'-C1'-C2'	2.18	108.04	105.79
1	A	105	UFT	C3'-C2'-C1'	-2.17	100.50	103.13
1	B	212	AF2	C5-C6-N1	-2.15	115.47	120.35
1	D	413[A]	UFT	C3'-C2'-C1'	-2.15	100.52	103.13
1	A	102	GF2	O6-C6-C5	2.15	128.56	124.37
1	E	506	UFT	C3'-C2'-C1'	-2.13	100.55	103.13
1	A	108	GF2	C2-N1-C6	-2.11	121.21	125.10
1	C	304	AF2	C5-C6-N1	-2.09	115.61	120.35
1	E	503	AF2	C5-C6-N1	-2.09	115.62	120.35
1	C	305	UFT	C3'-C2'-C1'	-2.09	100.60	103.13
1	E	508	GF2	O4'-C1'-C2'	2.09	107.94	105.79
1	B	213	UFT	O4-C4-C5	2.08	128.83	125.16
1	C	302	GF2	O6-C6-C5	2.07	128.42	124.37
1	A	108	GF2	O6-C6-C5	2.07	128.42	124.37
1	D	409[B]	CFZ	C3'-C2'-C1'	-2.07	100.62	103.13
1	B	214	UFT	O4'-C1'-C2'	2.07	107.92	105.79
1	C	308	GF2	O4'-C1'-C2'	2.06	107.92	105.79
1	D	414[A]	UFT	C2'-C1'-N1	-2.06	111.06	114.20
1	D	414[B]	UFT	C2'-C1'-N1	-2.06	111.06	114.20
1	C	306[A]	UFT	O3'-C3'-C2'	2.05	119.25	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	613	UFT	O4'-C1'-C2'	2.05	107.90	105.79
1	C	306[A]	UFT	O2-C2-N3	2.04	125.30	121.50
1	A	104	AF2	O4'-C1'-C2'	2.02	107.87	105.79
1	C	305	UFT	O2-C2-N3	2.00	125.23	121.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	306[B]	UFT	C3'-C4'-C5'-O5'
1	C	306[B]	UFT	O4'-C4'-C5'-O5'
1	C	306[A]	UFT	C3'-C4'-C5'-O5'
1	F	609	CFZ	C3'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	506	UFT	1	0
1	C	306[B]	UFT	1	0
1	E	502	GF2	1	0
1	E	505	UFT	1	0
1	A	104	AF2	1	0
1	E	501	CFZ	1	0
1	C	301	CFZ	1	0
1	B	213	UFT	2	0
1	B	209	CFZ	1	0
1	D	409[A]	CFZ	1	0
1	D	409[B]	CFZ	2	0
1	F	613	UFT	1	0
1	D	410[A]	GF2	1	0
1	F	612	AF2	1	0
1	D	410[B]	GF2	2	0
1	A	105	UFT	1	0
1	B	214	UFT	2	0
1	C	302	GF2	1	0
1	D	415	CFZ	1	0
1	B	210	GF2	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	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 [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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	UFT	D	414[A]	20/21	0.93	0.10	17,22,27,29	0
1	UFT	D	414[B]	20/21	0.93	0.10	17,22,26,35	5
1	UFT	C	306[A]	20/21	0.94	0.11	16,20,28,29	20
1	UFT	C	306[B]	20/21	0.94	0.11	16,21,30,31	20
1	CFZ	C	307[A]	20/21	0.95	0.09	10,15,26,26	5
1	CFZ	C	307[B]	20/21	0.95	0.09	10,15,27,30	5
1	CFZ	F	609	17/21	0.95	0.07	19,22,27,35	0
1	GF2	A	102	23/24	0.96	0.07	13,15,24,27	0
1	AF2	A	104	22/23	0.96	0.08	11,13,17,21	0
1	CFZ	D	415	20/21	0.96	0.08	10,15,27,31	0
1	CFZ	A	101	17/21	0.96	0.07	19,23,33,51	0
1	GF2	F	610	23/24	0.96	0.07	12,15,24,31	0
1	AF2	F	612	22/23	0.96	0.08	11,14,17,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	UFT	B	214	20/21	0.97	0.08	13,15,21,23	0
1	GF2	D	416	23/24	0.97	0.07	9,11,17,22	0
1	CFZ	E	501	17/21	0.97	0.07	10,12,15,19	0
1	AF2	E	503	22/23	0.97	0.07	11,12,14,16	0
1	UFT	E	505	20/21	0.97	0.08	14,16,19,19	0
1	UFT	E	506	20/21	0.97	0.07	13,14,23,24	0
1	GF2	B	216	23/24	0.97	0.07	15,17,20,22	0
1	AF2	A	103	22/23	0.97	0.06	12,15,18,23	0
1	AF2	F	611	22/23	0.97	0.07	12,14,18,22	0
1	UFT	B	213	20/21	0.97	0.06	13,16,19,20	0
1	GF2	C	308	23/24	0.98	0.06	8,11,18,21	0
1	CFZ	D	409[A]	17/21	0.98	0.07	9,10,12,13	17
1	CFZ	D	409[B]	17/21	0.98	0.07	8,11,18,18	17
1	AF2	D	412	22/23	0.98	0.07	11,15,22,23	0
1	UFT	D	413[A]	20/21	0.98	0.09	11,18,25,25	20
1	UFT	D	413[B]	20/21	0.98	0.09	13,20,28,29	20
1	UFT	A	106	20/21	0.98	0.06	10,12,18,19	0
1	CFZ	B	215	20/21	0.98	0.06	12,14,16,17	0
1	CFZ	B	209	17/21	0.98	0.06	10,12,16,19	0
1	CFZ	C	301	17/21	0.98	0.06	9,10,13,15	0
1	GF2	C	302	23/24	0.98	0.06	8,9,11,11	0
1	GF2	E	502	23/24	0.98	0.06	9,11,14,16	0
1	AF2	C	303	22/23	0.98	0.06	9,10,12,15	0
1	AF2	E	504	22/23	0.98	0.06	10,13,17,20	0
1	AF2	C	304	22/23	0.98	0.07	11,16,24,27	0
1	UFT	C	305	20/21	0.98	0.07	12,18,27,27	0
1	CFZ	E	507	20/21	0.98	0.06	11,14,16,16	0
1	GF2	E	508	23/24	0.98	0.07	16,17,21,24	0
1	GF2	B	210	23/24	0.98	0.07	9,12,14,16	0
1	AF2	B	211	22/23	0.98	0.06	10,12,14,16	0
1	AF2	B	212	22/23	0.98	0.06	10,13,17,18	0
1	UFT	A	105	20/21	0.98	0.07	10,11,20,21	0
1	UFT	F	613	20/21	0.98	0.07	9,11,20,21	0
1	UFT	F	614	20/21	0.98	0.06	11,12,18,18	0
1	GF2	D	410[B]	23/24	0.99	0.07	7,9,14,16	23
1	AF2	D	411[A]	22/23	0.99	0.06	8,10,11,12	5
1	AF2	D	411[B]	22/23	0.99	0.06	8,10,15,15	5
1	CFZ	A	107	20/21	0.99	0.06	9,12,15,17	0
1	GF2	A	108	23/24	0.99	0.05	8,9,12,14	0
1	GF2	D	410[A]	23/24	0.99	0.07	8,9,9,10	23
1	CFZ	F	615	20/21	0.99	0.06	9,11,14,17	0
1	GF2	F	616	23/24	0.99	0.05	8,9,13,15	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SR	E	709	1/1	0.97	0.14	28,28,28,28	1
2	SR	C	701	1/1	0.99	0.24	21,21,21,21	0
2	SR	D	702	1/1	0.99	0.22	20,20,20,20	0
2	SR	A	705	1/1	0.99	0.23	32,32,32,32	0
2	SR	F	706	1/1	0.99	0.28	18,18,18,18	1
3	MG	B	711	1/1	0.99	0.23	19,19,19,19	1
3	MG	E	712	1/1	0.99	0.25	21,21,21,21	1
2	SR	C	707	1/1	1.00	0.23	23,23,23,23	0
2	SR	B	704	1/1	1.00	0.14	18,18,18,18	1
2	SR	D	708	1/1	1.00	0.22	23,23,23,23	0
2	SR	E	703	1/1	1.00	0.15	18,18,18,18	1

6.5 Other polymers [i](#)

There are no such residues in this entry.