



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:02 PM BST

PDB ID : 3P4A
Title : 2'Fluoro modified RNA octamer fA2U2
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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 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 : 2.13.1
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) : 2.13.1

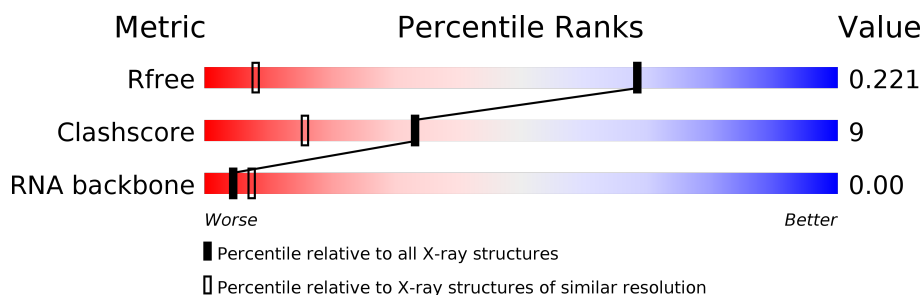
1 Overall quality at a glance

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 on 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	<div> <div>75%</div> <div>25%</div> </div>
1	B	8	<div> <div>50%</div> <div>50%</div> </div>
1	C	8	<div> <div>63%</div> <div>38%</div> </div>
1	D	8	<div> <div>63%</div> <div>38%</div> </div>
1	E	8	<div> <div>50%</div> <div>50%</div> </div>
1	F	8	<div> <div>75%</div> <div>25%</div> </div>

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

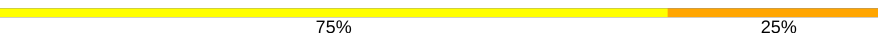
- Molecule 4 is water.

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, 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.

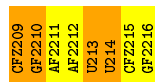
- Molecule 1: 2'Fluoro modified RNA 8-MER

Chain A: 

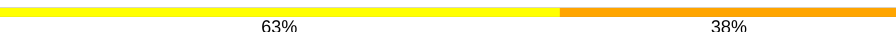


- Molecule 1: 2'Fluoro modified RNA 8-MER

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

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.60 (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	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: 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	GF2	F	616	1,2	18,25,26	1.29	1 (5%)	20,37,40	2.15	3 (15%)
1	GF2	D	410[A]	1	18,25,26	1.31	2 (11%)	20,37,40	2.47	4 (20%)
1	UFT	F	614	1	14,21,22	1.39	3 (21%)	14,30,33	1.65	3 (21%)
1	AF2	E	504	1	18,24,25	0.83	0	18,35,38	1.39	3 (16%)
1	GF2	D	410[B]	1	18,25,26	1.22	2 (11%)	20,37,40	2.51	5 (25%)
1	AF2	C	303	1	18,24,25	0.82	0	18,35,38	1.01	1 (5%)
1	GF2	F	610	1	18,25,26	1.33	2 (11%)	20,37,40	2.34	5 (25%)
1	CFZ	F	615	1	15,21,22	0.90	0	17,30,33	1.64	3 (17%)
1	CFZ	D	415	1	15,21,22	1.06	1 (6%)	17,30,33	1.72	2 (11%)
1	UFT	C	306[A]	1	14,21,22	1.27	1 (7%)	14,30,33	1.72	3 (21%)
1	UFT	B	213	1,2	14,21,22	1.19	1 (7%)	14,30,33	1.62	3 (21%)
1	AF2	D	412	1	18,24,25	0.79	0	18,35,38	1.60	4 (22%)
1	UFT	C	306[B]	1	14,21,22	1.16	1 (7%)	14,30,33	1.30	1 (7%)
1	CFZ	A	107	1	15,21,22	0.91	0	17,30,33	1.57	3 (17%)
1	UFT	A	106	1	14,21,22	1.22	2 (14%)	14,30,33	1.69	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	F	613	1	14,21,22	1.16	1 (7%)	14,30,33	1.45	3 (21%)
1	UFT	B	214	1	14,21,22	1.17	2 (14%)	14,30,33	1.57	4 (28%)
1	AF2	F	611	1	18,24,25	0.80	0	18,35,38	1.23	3 (16%)
1	CFZ	C	307[A]	1	15,21,22	0.90	0	17,30,33	1.60	2 (11%)
1	CFZ	B	209	1	15,18,22	1.03	1 (6%)	17,26,33	1.39	3 (17%)
1	CFZ	F	609	1	15,18,22	0.66	0	17,26,33	1.22	1 (5%)
1	UFT	E	506	1	14,21,22	1.01	1 (7%)	14,30,33	1.42	3 (21%)
1	UFT	D	414[A]	1	14,21,22	1.23	2 (14%)	14,30,33	2.15	4 (28%)
1	CFZ	C	307[B]	1	15,21,22	0.88	0	17,30,33	1.62	2 (11%)
1	CFZ	E	501	1	15,18,22	1.13	2 (13%)	17,26,33	1.62	4 (23%)
1	UFT	E	505	1,2	14,21,22	1.19	1 (7%)	14,30,33	1.54	2 (14%)
1	CFZ	D	409[B]	1	15,18,22	0.86	0	17,26,33	1.32	3 (17%)
1	GF2	A	108	1,2	18,25,26	1.56	3 (16%)	20,37,40	2.03	3 (15%)
1	UFT	D	414[B]	1	14,21,22	1.22	2 (14%)	14,30,33	2.13	4 (28%)
1	CFZ	D	409[A]	1	15,18,22	1.04	2 (13%)	17,26,33	1.58	2 (11%)
1	AF2	D	411[B]	1	18,24,25	0.84	1 (5%)	18,35,38	1.20	1 (5%)
1	CFZ	C	301	1	15,18,22	1.10	1 (6%)	17,26,33	1.85	3 (17%)
1	GF2	A	102	1	18,25,26	1.27	3 (16%)	20,37,40	2.52	4 (20%)
1	AF2	D	411[A]	1	18,24,25	0.83	1 (5%)	18,35,38	1.18	1 (5%)
1	UFT	A	105	1	14,21,22	1.03	1 (7%)	14,30,33	1.31	2 (14%)
1	AF2	E	503	1	18,24,25	0.86	1 (5%)	18,35,38	1.42	5 (27%)
1	GF2	C	308	1	18,25,26	1.20	2 (11%)	20,37,40	2.51	5 (25%)
1	GF2	E	502	1	18,25,26	1.74	4 (22%)	20,37,40	2.80	7 (35%)
1	GF2	B	216	1	18,25,26	1.29	2 (11%)	20,37,40	2.43	4 (20%)
1	CFZ	B	215	1	15,21,22	0.67	0	17,30,33	1.73	3 (17%)
1	GF2	D	416	1	18,25,26	1.38	2 (11%)	20,37,40	2.68	6 (30%)
1	AF2	B	211	1	18,24,25	0.85	1 (5%)	18,35,38	1.66	4 (22%)
1	CFZ	A	101	1	15,18,22	0.83	0	17,26,33	1.31	1 (5%)
1	GF2	C	302	1	18,25,26	1.21	1 (5%)	20,37,40	2.73	5 (25%)
1	UFT	D	413[B]	1	14,21,22	1.19	1 (7%)	14,30,33	1.43	3 (21%)
1	GF2	B	210	1	18,25,26	1.56	3 (16%)	20,37,40	2.64	6 (30%)
1	GF2	E	508	1	18,25,26	1.25	2 (11%)	20,37,40	2.53	5 (25%)
1	UFT	D	413[A]	1	14,21,22	1.26	2 (14%)	14,30,33	1.62	3 (21%)
1	AF2	A	104	1	18,24,25	0.91	1 (5%)	18,35,38	1.30	2 (11%)
1	AF2	A	103	1	18,24,25	0.74	1 (5%)	18,35,38	1.37	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AF2	B	212	1	18,24,25	0.91	1 (5%)	18,35,38	1.50	4 (22%)
1	CFZ	E	507	1	15,21,22	0.80	0	17,30,33	1.58	2 (11%)
1	AF2	C	304	1	18,24,25	0.81	0	18,35,38	1.35	4 (22%)
1	UFT	C	305	1	14,21,22	1.30	2 (14%)	14,30,33	1.65	3 (21%)
1	AF2	F	612	1	18,24,25	0.92	0	18,35,38	1.34	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GF2	F	616	1,2	-	0/3/25/26	0/3/3/3
1	GF2	D	410[A]	1	-	0/3/25/26	0/3/3/3
1	UFT	F	614	1	-	0/5/25/26	0/2/2/2
1	AF2	E	504	1	-	0/3/25/26	0/3/3/3
1	GF2	D	410[B]	1	-	0/3/25/26	0/3/3/3
1	AF2	C	303	1	-	0/3/25/26	0/3/3/3
1	GF2	F	610	1	-	0/3/25/26	0/3/3/3
1	CFZ	F	615	1	-	0/5/25/26	0/2/2/2
1	CFZ	D	415	1	-	0/5/25/26	0/2/2/2
1	UFT	C	306[A]	1	-	1/5/25/26	0/2/2/2
1	UFT	B	213	1,2	-	0/5/25/26	0/2/2/2
1	AF2	D	412	1	-	0/3/25/26	0/3/3/3
1	UFT	C	306[B]	1	-	2/5/25/26	0/2/2/2
1	CFZ	A	107	1	-	0/5/25/26	0/2/2/2
1	UFT	A	106	1	-	0/5/25/26	0/2/2/2
1	UFT	F	613	1	-	0/5/25/26	0/2/2/2
1	UFT	B	214	1	-	0/5/25/26	0/2/2/2
1	AF2	F	611	1	-	0/3/25/26	0/3/3/3
1	CFZ	C	307[A]	1	-	0/5/25/26	0/2/2/2
1	CFZ	B	209	1	-	0/4/22/26	0/2/2/2
1	CFZ	F	609	1	-	1/4/22/26	0/2/2/2
1	UFT	E	506	1	-	0/5/25/26	0/2/2/2
1	UFT	D	414[A]	1	-	0/5/25/26	0/2/2/2
1	CFZ	C	307[B]	1	-	0/5/25/26	0/2/2/2
1	CFZ	E	501	1	-	0/4/22/26	0/2/2/2
1	UFT	E	505	1,2	-	0/5/25/26	0/2/2/2
1	CFZ	D	409[B]	1	-	0/4/22/26	0/2/2/2
1	GF2	A	108	1,2	-	0/3/25/26	0/3/3/3
1	UFT	D	414[B]	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	D	409[A]	1	-	0/4/22/26	0/2/2/2
1	AF2	D	411[B]	1	-	0/3/25/26	0/3/3/3
1	CFZ	C	301	1	-	0/4/22/26	0/2/2/2
1	GF2	A	102	1	-	0/3/25/26	0/3/3/3
1	AF2	D	411[A]	1	-	0/3/25/26	0/3/3/3
1	UFT	A	105	1	-	0/5/25/26	0/2/2/2
1	AF2	E	503	1	-	0/3/25/26	0/3/3/3
1	GF2	C	308	1	-	0/3/25/26	0/3/3/3
1	GF2	E	502	1	-	0/3/25/26	0/3/3/3
1	GF2	B	216	1	-	0/3/25/26	0/3/3/3
1	CFZ	B	215	1	-	0/5/25/26	0/2/2/2
1	GF2	D	416	1	-	0/3/25/26	0/3/3/3
1	AF2	B	211	1	-	0/3/25/26	0/3/3/3
1	CFZ	A	101	1	-	0/4/22/26	0/2/2/2
1	GF2	C	302	1	-	0/3/25/26	0/3/3/3
1	UFT	D	413[B]	1	-	0/5/25/26	0/2/2/2
1	GF2	B	210	1	-	0/3/25/26	0/3/3/3
1	GF2	E	508	1	-	0/3/25/26	0/3/3/3
1	UFT	D	413[A]	1	-	0/5/25/26	0/2/2/2
1	AF2	A	104	1	-	0/3/25/26	0/3/3/3
1	AF2	A	103	1	-	0/3/25/26	0/3/3/3
1	AF2	B	212	1	-	0/3/25/26	0/3/3/3
1	CFZ	E	507	1	-	0/5/25/26	0/2/2/2
1	AF2	C	304	1	-	0/3/25/26	0/3/3/3
1	UFT	C	305	1	-	0/5/25/26	0/2/2/2
1	AF2	F	612	1	-	0/3/25/26	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GF2	C6-N1	5.07	1.41	1.33
1	E	502	GF2	O4'-C1'	4.57	1.47	1.41
1	F	610	GF2	C6-N1	4.34	1.40	1.33
1	E	502	GF2	C6-N1	4.28	1.40	1.33
1	F	616	GF2	C6-N1	4.27	1.40	1.33
1	D	410[A]	GF2	C6-N1	4.18	1.40	1.33
1	C	302	GF2	C6-N1	4.06	1.40	1.33
1	B	216	GF2	C6-N1	3.96	1.39	1.33
1	B	210	GF2	O4'-C1'	3.94	1.46	1.41
1	D	410[B]	GF2	C6-N1	3.92	1.39	1.33
1	A	102	GF2	C6-N1	3.88	1.39	1.33
1	E	508	GF2	C6-N1	3.79	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GF2	C6-N1	3.76	1.39	1.33
1	E	505	UFT	C4-N3	3.70	1.39	1.33
1	D	416	GF2	C6-N1	3.53	1.39	1.33
1	B	213	UFT	C4-N3	3.39	1.38	1.33
1	D	413[B]	UFT	C4-N3	3.26	1.38	1.33
1	D	413[A]	UFT	C4-N3	3.20	1.38	1.33
1	F	613	UFT	C4-N3	3.16	1.38	1.33
1	A	106	UFT	C4-N3	3.15	1.38	1.33
1	C	305	UFT	C4-N3	3.09	1.38	1.33
1	C	306[B]	UFT	C4-N3	3.04	1.38	1.33
1	C	308	GF2	O4'-C1'	3.01	1.45	1.41
1	C	306[A]	UFT	C4-N3	3.01	1.38	1.33
1	D	416	GF2	O4'-C1'	3.00	1.45	1.41
1	B	214	UFT	C4-N3	2.96	1.38	1.33
1	F	614	UFT	O4'-C1'	2.95	1.45	1.41
1	D	414[A]	UFT	C6-C5	-2.92	1.31	1.38
1	D	414[B]	UFT	C6-C5	-2.92	1.31	1.38
1	B	212	AF2	C8-N7	-2.78	1.29	1.34
1	D	414[A]	UFT	C4-N3	2.75	1.37	1.33
1	D	414[B]	UFT	C4-N3	2.75	1.37	1.33
1	C	308	GF2	C6-N1	2.73	1.37	1.33
1	C	301	CFZ	C2-N3	-2.63	1.33	1.38
1	A	105	UFT	C4-N3	2.58	1.37	1.33
1	F	614	UFT	C4-N3	2.56	1.37	1.33
1	E	506	UFT	C4-N3	2.55	1.37	1.33
1	F	614	UFT	C6-C5	-2.53	1.32	1.38
1	D	411[B]	AF2	C2-N3	2.52	1.36	1.32
1	D	411[A]	AF2	C2-N3	2.52	1.36	1.32
1	B	216	GF2	C8-N7	-2.48	1.30	1.34
1	E	502	GF2	C2'-C1'	-2.33	1.50	1.53
1	C	305	UFT	C6-N1	2.30	1.38	1.35
1	D	410[B]	GF2	C8-N7	-2.28	1.30	1.34
1	E	503	AF2	O4'-C1'	2.26	1.44	1.41
1	A	106	UFT	O4'-C1'	2.25	1.44	1.41
1	B	214	UFT	C6-N1	2.22	1.38	1.35
1	A	104	AF2	C4-N3	-2.22	1.32	1.35
1	E	501	CFZ	C6-C5	-2.18	1.33	1.38
1	A	102	GF2	C8-N7	-2.17	1.30	1.34
1	B	210	GF2	C2'-C1'	-2.17	1.50	1.53
1	A	108	GF2	O4'-C1'	2.16	1.44	1.41
1	B	209	CFZ	C6-C5	-2.14	1.33	1.38
1	F	610	GF2	C8-N7	-2.14	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	409[A]	CFZ	C2-N3	-2.14	1.33	1.38
1	D	415	CFZ	C4-N3	-2.12	1.32	1.35
1	D	410[A]	GF2	C8-N7	-2.09	1.31	1.34
1	E	502	GF2	C8-N7	-2.06	1.31	1.34
1	E	508	GF2	C8-N7	-2.06	1.31	1.34
1	D	413[A]	UFT	O4'-C1'	2.06	1.43	1.41
1	E	501	CFZ	O4'-C1'	2.03	1.43	1.41
1	A	102	GF2	C2-N1	2.03	1.39	1.35
1	A	103	AF2	F-C2'	-2.03	1.35	1.40
1	D	409[A]	CFZ	O4'-C1'	2.02	1.43	1.41
1	B	211	AF2	O4'-C1'	2.01	1.43	1.41
1	A	108	GF2	C8-N7	-2.00	1.31	1.34

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	508	GF2	C5-C6-N1	-8.86	111.31	123.43
1	B	210	GF2	C5-C6-N1	-8.47	111.85	123.43
1	D	416	GF2	C5-C6-N1	-8.40	111.94	123.43
1	D	410[B]	GF2	C5-C6-N1	-8.35	112.02	123.43
1	A	102	GF2	C5-C6-N1	-8.28	112.11	123.43
1	E	502	GF2	C5-C6-N1	-8.19	112.22	123.43
1	B	216	GF2	C5-C6-N1	-8.11	112.34	123.43
1	C	302	GF2	C5-C6-N1	-8.04	112.43	123.43
1	D	410[A]	GF2	C5-C6-N1	-7.99	112.50	123.43
1	C	308	GF2	C5-C6-N1	-7.98	112.52	123.43
1	F	610	GF2	C5-C6-N1	-7.42	113.28	123.43
1	F	616	GF2	C5-C6-N1	-7.37	113.35	123.43
1	A	108	GF2	C5-C6-N1	-7.20	113.58	123.43
1	C	302	GF2	C6-N1-C2	6.11	125.63	115.93
1	D	416	GF2	C6-N1-C2	5.74	125.06	115.93
1	C	301	CFZ	C2-N3-C4	5.60	122.01	116.34
1	C	308	GF2	C6-N1-C2	5.53	124.72	115.93
1	D	410[B]	GF2	C6-N1-C2	5.19	124.18	115.93
1	B	215	CFZ	C2-N3-C4	5.18	121.59	116.34
1	D	415	CFZ	C2-N3-C4	5.09	121.50	116.34
1	F	615	CFZ	C2-N3-C4	5.05	121.46	116.34
1	E	502	GF2	C6-N1-C2	4.92	123.75	115.93
1	B	210	GF2	C6-N1-C2	4.76	123.49	115.93
1	A	102	GF2	C6-N1-C2	4.72	123.42	115.93
1	B	216	GF2	C6-N1-C2	4.71	123.42	115.93
1	D	410[A]	GF2	C6-N1-C2	4.70	123.39	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	508	GF2	C6-N1-C2	4.68	123.37	115.93
1	C	307[A]	CFZ	C2-N3-C4	4.59	120.99	116.34
1	C	307[B]	CFZ	C2-N3-C4	4.59	120.99	116.34
1	E	507	CFZ	C2-N3-C4	4.49	120.89	116.34
1	A	107	CFZ	C2-N3-C4	4.45	120.86	116.34
1	D	409[A]	CFZ	C2-N3-C4	4.29	120.69	116.34
1	F	610	GF2	C6-N1-C2	4.27	122.72	115.93
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
1	B	212	AF2	C5-C6-N6	4.19	126.71	120.35
1	B	213	UFT	C5-C4-N3	-4.06	114.37	123.31
1	F	614	UFT	C5-C4-N3	-4.05	114.39	123.31
1	C	306[B]	UFT	C5-C4-N3	-4.00	114.52	123.31
1	D	414[A]	UFT	C5-C4-N3	-3.94	114.63	123.31
1	D	414[B]	UFT	C5-C4-N3	-3.94	114.63	123.31
1	C	302	GF2	N3-C2-N1	-3.94	121.97	127.22
1	F	616	GF2	C6-N1-C2	3.89	122.11	115.93
1	B	214	UFT	C5-C4-N3	-3.87	114.80	123.31
1	C	305	UFT	C5-C4-N3	-3.83	114.89	123.31
1	A	102	GF2	C2-N3-C4	-3.82	110.99	115.36
1	D	413[B]	UFT	C5-C4-N3	-3.78	114.99	123.31
1	D	413[A]	UFT	C5-C4-N3	-3.77	115.01	123.31
1	E	505	UFT	C5-C4-N3	-3.72	115.13	123.31
1	E	502	GF2	O4'-C1'-C2'	3.69	109.59	105.79
1	A	105	UFT	C5-C4-N3	-3.60	115.39	123.31
1	B	210	GF2	C2-N3-C4	-3.57	111.28	115.36
1	E	501	CFZ	O4'-C1'-C2'	3.56	109.46	105.79
1	A	106	UFT	C5-C4-N3	-3.55	115.50	123.31
1	D	409[B]	CFZ	C2-N3-C4	3.51	119.90	116.34
1	E	501	CFZ	F2'-C2'-C1'	-3.51	101.76	109.08
1	F	613	UFT	C5-C4-N3	-3.49	115.62	123.31
1	F	609	CFZ	C2-N3-C4	3.45	119.84	116.34
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	A	108	GF2	C6-N1-C2	3.32	121.21	115.93
1	E	502	GF2	C2-N3-C4	-3.31	111.58	115.36
1	D	412	AF2	O4'-C1'-C2'	3.30	109.19	105.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	GF2	N3-C2-N1	-3.28	122.85	127.22
1	A	101	CFZ	C2-N3-C4	3.24	119.62	116.34
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	416	GF2	C2-N3-C4	-3.12	111.80	115.36
1	D	410[A]	GF2	C2-N3-C4	-3.11	111.81	115.36
1	D	413[A]	UFT	O4'-C1'-C2'	3.11	108.99	105.79
1	C	306[A]	UFT	C5-C4-N3	-3.08	116.54	123.31
1	E	506	UFT	C5-C4-N3	-3.05	116.60	123.31
1	E	504	AF2	C3'-C2'-C1'	-3.02	99.48	103.13
1	E	508	GF2	C2-N3-C4	-2.99	111.94	115.36
1	F	611	AF2	C3'-C2'-C1'	-2.99	99.51	103.13
1	E	501	CFZ	C2-N3-C4	2.96	119.34	116.34
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[B]	AF2	C3'-C2'-C1'	-2.92	99.59	103.13
1	D	411[A]	AF2	C3'-C2'-C1'	-2.92	99.59	103.13
1	B	212	AF2	C3'-C2'-C1'	-2.92	99.60	103.13
1	B	216	GF2	C2-N3-C4	-2.91	112.03	115.36
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	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	416	GF2	N3-C2-N1	-2.89	123.37	127.22
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
1	C	302	GF2	C6-C5-C4	-2.73	118.19	120.80
1	B	210	GF2	C3'-C2'-C1'	-2.73	99.83	103.13
1	C	301	CFZ	F2'-C2'-C1'	-2.66	103.54	109.08
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	502	GF2	C4-C5-N7	2.60	112.11	109.40
1	C	302	GF2	C3'-C2'-C1'	-2.59	100.00	103.13
1	B	211	AF2	C5-C6-N6	2.58	124.27	120.35
1	F	610	GF2	C6-C5-C4	-2.56	118.35	120.80
1	F	616	GF2	C2-N3-C4	-2.53	112.46	115.36
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	505	UFT	C6-N1-C2	-2.46	117.29	121.20
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	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	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	A	107	CFZ	N4-C4-N3	2.37	120.24	116.49
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	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
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	D	410[B]	GF2	C2-N3-C4	-2.33	112.69	115.36
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	D	416	GF2	C6-C5-C4	-2.30	118.60	120.80
1	B	214	UFT	F2'-C2'-C1'	-2.30	104.29	109.08
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	D	410[B]	GF2	N3-C2-N1	-2.26	124.21	127.22
1	F	612	AF2	O4'-C1'-C2'	2.24	108.10	105.79
1	A	102	GF2	C3'-C2'-C1'	-2.21	100.45	103.13
1	D	413[B]	UFT	F2'-C2'-C3'	-2.21	104.59	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	612	AF2	N3-C2-N1	-2.20	125.25	128.68
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	E	506	UFT	C3'-C2'-C1'	-2.13	100.55	103.13
1	D	415	CFZ	N4-C4-N3	2.10	119.82	116.49
1	C	304	AF2	C5-C6-N1	-2.09	115.61	120.35
1	B	213	UFT	C6-N1-C2	-2.09	117.88	121.20
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	C	308	GF2	C2-N3-C4	-2.08	112.98	115.36
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	F	610	GF2	C2-N3-C4	-2.07	112.99	115.36
1	A	108	GF2	C6-C5-C4	-2.07	118.82	120.80
1	C	308	GF2	O4'-C1'-C2'	2.06	107.92	105.79
1	C	306[A]	UFT	O3'-C3'-C2'	2.05	119.25	111.57
1	F	613	UFT	O4'-C1'-C2'	2.05	107.90	105.79
1	A	104	AF2	O4'-C1'-C2'	2.02	107.87	105.79
1	F	615	CFZ	N4-C4-N3	2.01	119.67	116.49

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	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	B	213	UFT	2	0
1	C	306[B]	UFT	1	0
1	F	613	UFT	1	0
1	B	214	UFT	2	0
1	B	209	CFZ	1	0
1	E	506	UFT	1	0
1	E	501	CFZ	1	0
1	E	505	UFT	1	0
1	D	409[B]	CFZ	2	0
1	D	409[A]	CFZ	1	0
1	C	301	CFZ	1	0
1	A	105	UFT	1	0
1	E	502	GF2	1	0
1	C	302	GF2	1	0
1	B	210	GF2	1	0
1	A	104	AF2	1	0
1	F	612	AF2	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 ⓘ

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	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. 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	CFZ	D	415	20/21	0.96	0.08	10,15,27,31	0
1	GF2	F	610	23/24	0.96	0.07	12,15,24,31	0
1	GF2	A	102	23/24	0.96	0.07	13,15,24,27	0
1	CFZ	A	101	17/21	0.96	0.07	19,23,33,51	0
1	AF2	A	104	22/23	0.96	0.08	11,13,17,21	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	CFZ	E	501	17/21	0.97	0.07	10,12,15,19	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	AF2	E	503	22/23	0.97	0.07	11,12,14,16	0
1	GF2	B	216	23/24	0.97	0.07	15,17,20,22	0
1	GF2	D	416	23/24	0.97	0.07	9,11,17,22	0
1	UFT	E	506	20/21	0.97	0.07	13,14,23,24	0
1	AF2	A	103	22/23	0.97	0.06	12,15,18,23	0
1	UFT	E	505	20/21	0.97	0.08	14,16,19,19	0
1	CFZ	D	409[B]	17/21	0.98	0.07	8,11,18,18	17
1	AF2	C	303	22/23	0.98	0.06	9,10,12,15	0
1	CFZ	D	409[A]	17/21	0.98	0.07	9,10,12,13	17
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	CFZ	B	209	17/21	0.98	0.06	10,12,16,19	0
1	UFT	C	305	20/21	0.98	0.07	12,18,27,27	0
1	UFT	F	614	20/21	0.98	0.06	11,12,18,18	0
1	GF2	C	308	23/24	0.98	0.06	8,11,18,21	0
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	UFT	F	613	20/21	0.98	0.07	9,11,20,21	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	E	504	22/23	0.98	0.06	10,13,17,20	0
1	AF2	D	412	22/23	0.98	0.07	11,15,22,23	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
1	UFT	A	105	20/21	0.98	0.07	10,11,20,21	0
1	CFZ	A	107	20/21	0.99	0.06	9,12,15,17	0
1	AF2	D	411[B]	22/23	0.99	0.06	8,10,15,15	5
1	CFZ	F	615	20/21	0.99	0.06	9,11,14,17	0
1	GF2	D	410[B]	23/24	0.99	0.07	7,9,14,16	23
1	GF2	F	616	23/24	0.99	0.05	8,9,13,15	0
1	AF2	D	411[A]	22/23	0.99	0.06	8,10,11,12	5
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

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(\AA^2)	Q<0.9
2	SR	E	709	1/1	0.97	0.14	28,28,28,28	1
2	SR	F	706	1/1	0.99	0.28	18,18,18,18	1
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	D	702	1/1	0.99	0.22	20,20,20,20	0
3	MG	B	711	1/1	0.99	0.23	19,19,19,19	1
2	SR	D	708	1/1	1.00	0.22	23,23,23,23	0
2	SR	B	704	1/1	1.00	0.14	18,18,18,18	1
2	SR	E	703	1/1	1.00	0.15	18,18,18,18	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.