



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 05:02 AM EDT

PDB ID : 5SWM  
Title : BACILLUS HALODURANS RNASE H MUTANT D132N IN COMPLEX WITH 12-MER FRNA/DNA HYBRID  
Authors : Pallan, P.S.; Egli, M.  
Deposited on : 2016-08-08  
Resolution : 1.50 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

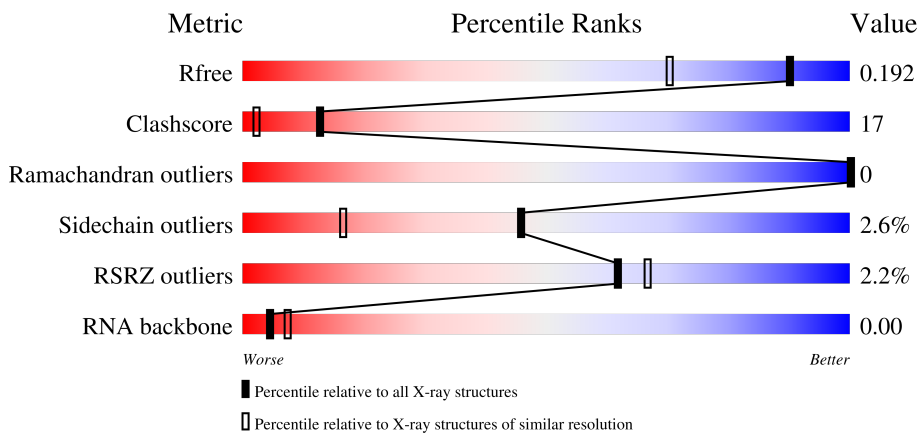
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)
RNA backbone	3102	1015 (2.36-0.86)

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  $\geq 3$ , 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	142	 4% 76% 14% • 8%
1	B	142	 % 78% 14% • 6%
2	C	12	 8% 92%
3	D	12	 8% 50% 33% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CFZ	C	12[C]	-	-	X	-
2	AF2	C	4[C]	-	-	X	-
2	CFZ	C	6[C]	-	-	X	-
2	UFT	C	7[C]	-	-	X	-
6	PEG	A	203	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3908 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 protein called Ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	1060	681	179	199	1	0	0	0
1	B	133	1073	688	181	203	1	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLY	-	expression tag	UNP Q9KEI9
A	56	SER	-	expression tag	UNP Q9KEI9
A	57	HIS	-	expression tag	UNP Q9KEI9
A	58	MET	-	expression tag	UNP Q9KEI9
A	132	ASN	ASP	engineered mutation	UNP Q9KEI9
B	55	GLY	-	expression tag	UNP Q9KEI9
B	56	SER	-	expression tag	UNP Q9KEI9
B	57	HIS	-	expression tag	UNP Q9KEI9
B	58	MET	-	expression tag	UNP Q9KEI9
B	132	ASN	ASP	engineered mutation	UNP Q9KEI9

- Molecule 2 is a RNA chain called RNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	F	N	O				P
2	C	12	747	339	36	129	210	33	0	12	0

- Molecule 3 is a DNA chain called DNA (12-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	Br	C	N	O				P
3	D	12	738	3	351	141	210	33	0	12	0

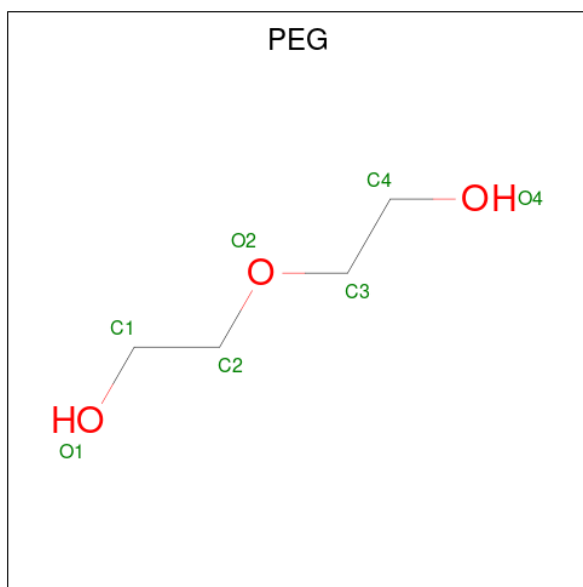
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 6 3 3	0	0

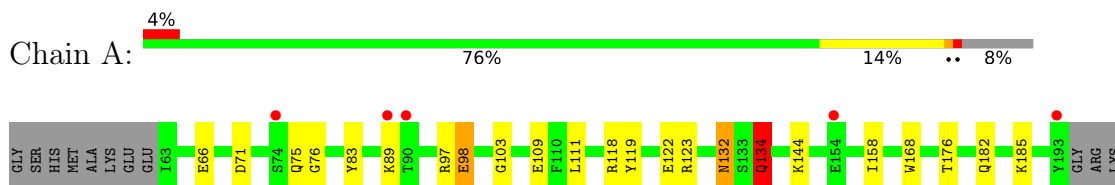
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	99	Total O 99 99	0	0
8	B	110	Total O 110 110	0	0
8	C	32	Total O 32 32	0	0
8	D	34	Total O 34 34	0	0

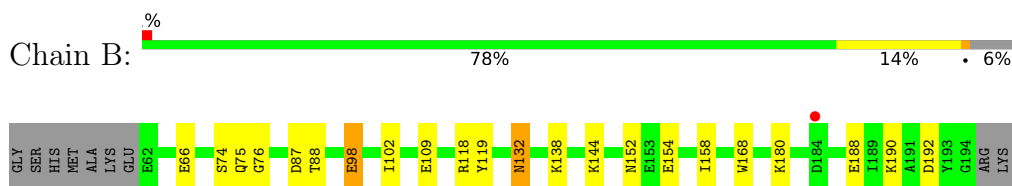
### 3 Residue-property plots [i](#)

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: Ribonuclease H



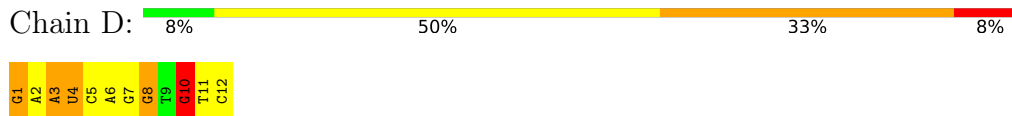
- Molecule 1: Ribonuclease H



- Molecule 2: RNA (12-MER)



- Molecule 3: DNA (12-MER)



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.47Å 44.50Å 62.17Å 84.42° 89.90° 65.10°	Depositor
Resolution (Å)	26.60 – 1.50 32.14 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (26.60-1.50) 95.3 (32.14-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.161 , 0.185 0.168 , 0.192	Depositor DCC
$R_{free}$ test set	2680 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtrriage
Anisotropy	0.503	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.449 for h,h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.32% 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, 0.333 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: AF2, UFT, GF2, NA, GOL, PEG, BRU, CFZ, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.29	6/1085 (0.6%)	0.79	0/1472
1	B	1.25	5/1098 (0.5%)	0.79	0/1489
3	D	1.14	3/759 (0.4%)	0.87	0/1161
All	All	1.24	14/2942 (0.5%)	0.81	0/4122

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
3	D	0	4
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	GLU	CD-OE1	-9.12	1.15	1.25
1	A	66	GLU	CD-OE2	-8.71	1.16	1.25
1	A	98	GLU	CD-OE2	-7.70	1.17	1.25
1	A	109	GLU	CD-OE2	6.67	1.32	1.25
1	A	71	ASP	CB-CG	6.26	1.65	1.51
1	A	119	TYR	CG-CD2	-6.03	1.31	1.39
1	B	66	GLU	CD-OE2	-5.37	1.19	1.25
1	B	109	GLU	CD-OE2	5.28	1.31	1.25
3	D	10[A]	DG	O3'-P	5.20	1.67	1.61
3	D	10[B]	DG	O3'-P	5.20	1.67	1.61
3	D	10[C]	DG	O3'-P	5.20	1.67	1.61
1	B	119	TYR	CG-CD1	-5.17	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	TYR	CE2-CZ	-5.16	1.31	1.38
1	A	134	GLN	CG-CD	-5.06	1.39	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLU	Sidechain
1	B	87	ASP	Sidechain
1	B	98	GLU	Sidechain
3	D	1[A]	DG	Sidechain
3	D	10[A]	DG	Sidechain
3	D	3[A]	DA	Sidechain
3	D	8[A]	DG	Sidechain

## 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	1060	0	1056	18	0
1	B	1073	0	1065	18	0
2	C	747	0	348	59	0
3	D	738	0	396	31	0
4	A	1	0	0	0	0
5	A	1	0	0	1	0
6	A	7	0	10	6	0
7	D	6	0	8	2	0
8	A	99	0	0	3	0
8	B	110	0	0	3	0
8	C	32	0	0	1	0
8	D	34	0	0	4	0
All	All	3908	0	2883	107	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 17.

All (107) 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)
2:C:6[C]:CFZ:C2'	2:C:7[C]:UFT:H5'A	1.66	1.22
2:C:6[C]:CFZ:H6	2:C:6[C]:CFZ:C5'	1.78	1.13
2:C:6[C]:CFZ:H2'	2:C:7[C]:UFT:H5'A	1.06	1.05
2:C:6[C]:CFZ:H6	2:C:6[C]:CFZ:H5'	1.00	0.99
2:C:7[C]:UFT:H6	2:C:7[C]:UFT:C5'	1.92	0.99
1:B:188:GLU:HG2	8:B:201:HOH:O	1.63	0.99
2:C:7[C]:UFT:H6	2:C:7[C]:UFT:H5'	1.43	0.99
3:D:7[B]:DG:H2'	3:D:8[B]:DG:C8	2.00	0.97
2:C:6[C]:CFZ:H2'	2:C:7[C]:UFT:C5'	1.96	0.96
3:D:1[C]:DG:H2''	3:D:2[C]:DA:O5'	1.67	0.94
2:C:6[C]:CFZ:H5'	2:C:6[C]:CFZ:C6	1.96	0.93
2:C:4[C]:AF2:H2	2:C:5[C]:CFZ:C2	2.04	0.88
1:A:75:GLN:HG3	2:C:7[C]:UFT:OP1	1.74	0.86
3:D:7[C]:DG:H2''	3:D:8[C]:DG:H5''	1.60	0.83
2:C:6[C]:CFZ:C3'	2:C:7[C]:UFT:H5'A	2.09	0.81
3:D:7[B]:DG:H2'	3:D:8[B]:DG:H8	1.46	0.80
2:C:4[C]:AF2:C2	2:C:5[C]:CFZ:C2	2.60	0.80
1:B:74:SER:HB2	2:C:12[C]:CFZ:C5'	2.15	0.76
1:B:74:SER:HB2	2:C:12[C]:CFZ:H5'	1.68	0.74
3:D:10[A]:DG:H2''	3:D:11[A]:DT:H5'	1.70	0.71
2:C:7[B]:UFT:OP2	8:C:101:HOH:O	2.08	0.70
3:D:4[C]:BRU:O4	3:D:5[C]:DC:N4	2.25	0.70
2:C:8[C]:GF2:C2	3:D:6[C]:DA:C2	2.76	0.69
1:B:192:ASP:OD2	8:B:201:HOH:O	2.10	0.68
2:C:6[C]:CFZ:C5'	2:C:6[C]:CFZ:C6	2.65	0.67
1:B:188:GLU:CG	8:B:201:HOH:O	2.33	0.65
1:A:132:ASN:O	2:C:5[A]:CFZ:H5'A	1.97	0.65
1:A:76:GLY:HA2	2:C:6[C]:CFZ:F2'	1.88	0.64
2:C:3[C]:CFZ:C4	2:C:4[C]:AF2:N7	2.60	0.64
2:C:6[C]:CFZ:C2'	2:C:7[C]:UFT:C5'	2.61	0.64
3:D:7[B]:DG:C2'	3:D:8[B]:DG:C8	2.79	0.63
2:C:7[C]:UFT:H6	2:C:7[C]:UFT:C4'	2.28	0.62
6:A:203:PEG:H31	8:A:337:HOH:O	1.99	0.62
1:A:83:TYR:OH	6:A:203:PEG:H22	2.00	0.61
2:C:4[C]:AF2:H1'	3:D:10[C]:DG:N2	2.15	0.61
3:D:7[B]:DG:C2'	3:D:8[B]:DG:H8	2.13	0.61
1:B:138:LYS:HE3	3:D:6[A]:DA:OP2	2.01	0.61
6:A:203:PEG:C3	8:A:337:HOH:O	2.48	0.60
1:A:97:ARG:HD3	6:A:203:PEG:H21	1.84	0.59
1:B:88:THR:O	1:B:190:LYS:CD	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4[C]:BRU:C4	3:D:5[C]:DC:N4	2.66	0.59
3:D:4[C]:BRU:C4	3:D:5[C]:DC:C4	2.86	0.58
3:D:7[C]:DG:C2'	3:D:8[C]:DG:H5''	2.31	0.58
1:B:74:SER:HB2	2:C:12[C]:CFZ:H5'A	1.86	0.57
1:A:132:ASN:C	1:A:132:ASN:HD22	2.07	0.57
3:D:10[C]:DG:OP2	8:D:201:HOH:O	2.14	0.56
1:B:132:ASN:C	1:B:132:ASN:HD22	2.08	0.55
2:C:8[C]:GF2:N2	3:D:6[C]:DA:C2	2.74	0.55
1:A:182:GLN:HE22	1:A:185:LYS:NZ	2.05	0.54
2:C:8[C]:GF2:C2	3:D:6[C]:DA:N1	2.69	0.54
3:D:6[A]:DA:H2''	3:D:7[A]:DG:H5''	1.89	0.54
2:C:4[C]:AF2:C2	2:C:5[C]:CFZ:N3	2.70	0.54
2:C:4[C]:AF2:H2	2:C:5[C]:CFZ:O2	2.08	0.53
1:B:88:THR:O	1:B:190:LYS:HD2	2.07	0.53
2:C:9[A]:AF2:H2'	2:C:10[A]:UFT:H6	1.90	0.53
2:C:10[C]:UFT:N3	2:C:11[C]:UFT:C5	2.71	0.53
2:C:12[C]:CFZ:H1'	7:D:101:GOL:H32	1.90	0.53
1:A:122:GLU:CG	1:A:123:ARG:NH1	2.71	0.53
1:A:75:GLN:HA	2:C:7[C]:UFT:OP1	2.11	0.51
2:C:2[B]:AF2:H8	2:C:2[B]:AF2:O5'	2.10	0.51
2:C:3[C]:CFZ:C4	2:C:4[C]:AF2:C8	2.88	0.51
2:C:6[C]:CFZ:C2	3:D:7[C]:DG:H22	2.24	0.51
2:C:7[C]:UFT:H2'	2:C:8[C]:GF2:O4'	2.11	0.50
2:C:4[C]:AF2:N1	2:C:5[C]:CFZ:N3	2.61	0.49
1:B:118:ARG:HG2	1:B:168:TRP:CE2	2.48	0.48
3:D:11[B]:DT:H73	8:D:215:HOH:O	2.11	0.48
1:A:103:GLY:HA3	1:A:158:ILE:HD13	1.95	0.48
1:A:118:ARG:HG2	1:A:168:TRP:CE2	2.49	0.47
2:C:6[C]:CFZ:C3'	2:C:7[C]:UFT:C5'	2.89	0.46
3:D:1[C]:DG:C2'	3:D:2[C]:DA:O5'	2.50	0.45
1:A:134:GLN:NE2	3:D:11[A]:DT:H4'	2.31	0.45
3:D:10[C]:DG:H2''	3:D:11[C]:DT:H5''	1.97	0.45
3:D:4[C]:BRU:N3	3:D:5[C]:DC:C4	2.85	0.45
2:C:3[C]:CFZ:N3	2:C:4[C]:AF2:C8	2.79	0.45
6:A:203:PEG:H32	8:A:337:HOH:O	2.14	0.45
7:D:101:GOL:H11	8:D:221:HOH:O	2.17	0.45
1:B:74:SER:C	2:C:12[C]:CFZ:H5'	2.38	0.44
2:C:8[B]:GF2:H2'	2:C:9[B]:AF2:O4'	2.18	0.44
1:B:180:LYS:NZ	2:C:10[C]:UFT:OP1	2.50	0.44
2:C:6[C]:CFZ:H6	2:C:6[C]:CFZ:C4'	2.41	0.44
2:C:9[B]:AF2:H2'	2:C:10[B]:UFT:H6	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12[B]:DC:H6	8:D:227:HOH:O	1.99	0.44
1:A:111:LEU:HD22	6:A:203:PEG:H32	1.99	0.43
2:C:8[C]:GF2:H2'	2:C:9[C]:AF2:H8	2.00	0.43
1:B:152:ASN:OD1	1:B:154:GLU:HB3	2.18	0.43
1:A:76:GLY:CA	2:C:6[C]:CFZ:F2'	2.56	0.43
1:B:76:GLY:N	2:C:12[C]:CFZ:H4'	2.35	0.42
2:C:5[C]:CFZ:O5'	2:C:5[C]:CFZ:H6	2.19	0.42
3:D:6[A]:DA:C4	3:D:7[A]:DG:C8	3.07	0.42
1:B:75:GLN:HA	2:C:12[C]:CFZ:O3'	2.19	0.42
2:C:2[C]:AF2:F	2:C:3[C]:CFZ:H5'A	2.10	0.42
2:C:6[C]:CFZ:O2	3:D:7[C]:DG:N2	2.50	0.42
2:C:7[C]:UFT:C4'	2:C:7[C]:UFT:C6	2.97	0.42
1:A:134:GLN:HE22	3:D:11[A]:DT:C4'	2.33	0.42
1:B:102:ILE:HG13	1:B:154:GLU:CG	2.50	0.41
1:B:76:GLY:HA2	2:C:12[C]:CFZ:F2'	2.10	0.41
2:C:11[B]:UFT:H2'	2:C:12[B]:CFZ:H6	2.02	0.41
1:A:134:GLN:HE22	3:D:11[A]:DT:H4'	1.85	0.41
1:A:176:THR:OG1	5:A:202:CL:CL	2.74	0.41
2:C:10[C]:UFT:H2'	2:C:11[C]:UFT:H6	2.02	0.41
2:C:11[B]:UFT:H2'	2:C:12[B]:CFZ:C6	2.50	0.41
3:D:2[C]:DA:H2''	3:D:3[C]:DA:H5'	2.03	0.41
3:D:1[B]:DG:H2'	3:D:2[B]:DA:C8	2.55	0.41
2:C:3[B]:CFZ:H6	2:C:3[B]:CFZ:O5'	2.21	0.40
2:C:10[C]:UFT:C2	2:C:11[C]:UFT:C6	2.99	0.40
1:A:89:LYS:HB3	1:A:89:LYS:HE3	1.89	0.40
2:C:11[C]:UFT:F2'	2:C:12[C]:CFZ:H5'A	2.12	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/142 (91%)	129 (100%)	0	0	100	100
1	B	131/142 (92%)	131 (100%)	0	0	100	100
All	All	260/284 (92%)	260 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/124 (92%)	111 (97%)	3 (3%)	46	16
1	B	115/124 (93%)	112 (97%)	3 (3%)	46	16
All	All	229/248 (92%)	223 (97%)	6 (3%)	46	16

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	134	GLN
1	A	144	LYS
1	B	132	ASN
1	B	144	LYS
1	B	158	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	182	GLN
1	B	132	ASN
1	B	170	ASN
1	B	182	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	0/12	-	-

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](#)

39 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
2	UFT	C	10[A]	3,2	18,21,22	1.52	4 (22%)	26,30,33	1.75	6 (23%)
2	UFT	C	11[A]	3,2	18,21,22	1.40	1 (5%)	26,30,33	2.03	5 (19%)
2	AF2	C	9[B]	2	18,24,25	1.44	3 (16%)	18,35,38	1.56	4 (22%)
2	AF2	C	9[C]	2	18,24,25	1.12	2 (11%)	18,35,38	1.44	1 (5%)
2	CFZ	C	6[A]	3,2	18,21,22	1.12	2 (11%)	26,30,33	1.35	4 (15%)
2	UFT	C	10[B]	2	18,21,22	1.70	4 (22%)	26,30,33	1.82	7 (26%)
2	UFT	C	11[B]	2	18,21,22	2.15	4 (22%)	26,30,33	2.05	7 (26%)
2	UFT	C	10[C]	2	18,21,22	1.47	3 (16%)	26,30,33	1.87	5 (19%)
2	UFT	C	11[C]	2	18,21,22	1.58	4 (22%)	26,30,33	2.05	9 (34%)
2	CFZ	C	6[B]	2	18,21,22	1.41	5 (27%)	26,30,33	1.58	4 (15%)
2	AF2	C	4[A]	3,2	18,24,25	1.17	2 (11%)	18,35,38	1.50	3 (16%)
2	CFZ	C	6[C]	2	18,21,22	1.87	2 (11%)	26,30,33	1.19	3 (11%)
2	GF2	C	1[A]	3,2	18,22,26	1.25	3 (16%)	19,33,40	1.11	1 (5%)
2	CFZ	C	5[A]	3,2	18,21,22	1.41	3 (16%)	26,30,33	1.60	4 (15%)
2	AF2	C	2[A]	3,2	18,24,25	1.30	2 (11%)	18,35,38	1.49	4 (22%)
2	AF2	C	4[B]	2	18,24,25	1.31	1 (5%)	18,35,38	1.66	4 (22%)
2	CFZ	C	3[A]	3,2	18,21,22	1.14	2 (11%)	26,30,33	1.03	1 (3%)
2	AF2	C	4[C]	2	18,24,25	1.23	1 (5%)	18,35,38	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GF2	C	1[B]	2	18,22,26	1.19	1 (5%)	19,33,40	1.30	3 (15%)
2	UFT	C	7[A]	3,2	18,21,22	1.83	5 (27%)	26,30,33	1.82	6 (23%)
2	CFZ	C	5[B]	2	18,21,22	1.15	2 (11%)	26,30,33	1.13	1 (3%)
2	AF2	C	2[B]	2	18,24,25	1.30	2 (11%)	18,35,38	1.64	3 (16%)
2	GF2	C	1[C]	2	18,22,26	1.63	4 (22%)	19,33,40	1.24	3 (15%)
2	CFZ	C	3[B]	2	18,21,22	1.20	3 (16%)	26,30,33	0.76	0
2	CFZ	C	5[C]	2	18,21,22	1.06	0	26,30,33	1.13	1 (3%)
2	CFZ	C	12[A]	3,2	18,21,22	1.42	3 (16%)	26,30,33	1.06	2 (7%)
3	BRU	D	4[A]	3,2	18,21,22	1.65	5 (27%)	26,30,33	1.68	6 (23%)
2	AF2	C	2[C]	2	18,24,25	1.60	3 (16%)	18,35,38	1.42	3 (16%)
2	UFT	C	7[B]	2	18,21,22	1.52	5 (27%)	26,30,33	1.91	7 (26%)
2	CFZ	C	3[C]	2	18,21,22	1.29	3 (16%)	26,30,33	1.04	1 (3%)
2	GF2	C	8[A]	3,2	18,25,26	1.48	5 (27%)	19,37,40	1.18	2 (10%)
2	UFT	C	7[C]	2	18,21,22	1.83	4 (22%)	26,30,33	1.94	8 (30%)
3	BRU	D	4[B]	3	18,21,22	1.82	4 (22%)	26,30,33	1.98	9 (34%)
2	CFZ	C	12[B]	2	18,21,22	1.33	3 (16%)	26,30,33	1.18	2 (7%)
3	BRU	D	4[C]	3	18,21,22	1.78	5 (27%)	26,30,33	2.30	9 (34%)
2	CFZ	C	12[C]	2	18,21,22	1.49	3 (16%)	26,30,33	1.08	3 (11%)
2	GF2	C	8[B]	2	18,25,26	0.99	1 (5%)	19,37,40	1.11	0
2	AF2	C	9[A]	3,2	18,24,25	1.66	4 (22%)	18,35,38	1.99	4 (22%)
2	GF2	C	8[C]	2	18,25,26	1.44	4 (22%)	19,37,40	1.31	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
2	UFT	C	10[A]	3,2	-	0/7/25/26	0/2/2/2
2	UFT	C	11[A]	3,2	-	2/7/25/26	0/2/2/2
2	AF2	C	9[B]	2	-	2/3/25/26	0/3/3/3
2	AF2	C	9[C]	2	-	0/3/25/26	0/3/3/3
2	CFZ	C	6[A]	3,2	-	0/7/25/26	0/2/2/2
2	UFT	C	10[B]	2	-	0/7/25/26	0/2/2/2
2	UFT	C	11[B]	2	-	2/7/25/26	0/2/2/2
2	UFT	C	10[C]	2	-	2/7/25/26	0/2/2/2
2	UFT	C	11[C]	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CFZ	C	6[B]	2	-	0/7/25/26	0/2/2/2
2	AF2	C	4[A]	3,2	-	0/3/25/26	0/3/3/3
2	CFZ	C	6[C]	2	-	2/7/25/26	0/2/2/2
2	GF2	C	1[A]	3,2	-	0/2/22/26	0/3/3/3
2	CFZ	C	5[A]	3,2	-	2/7/25/26	0/2/2/2
2	AF2	C	2[A]	3,2	-	0/3/25/26	0/3/3/3
2	AF2	C	4[B]	2	-	0/3/25/26	0/3/3/3
2	CFZ	C	3[A]	3,2	-	0/7/25/26	0/2/2/2
2	AF2	C	4[C]	2	-	0/3/25/26	0/3/3/3
2	GF2	C	1[B]	2	-	0/2/22/26	0/3/3/3
2	UFT	C	7[A]	3,2	-	1/7/25/26	0/2/2/2
2	CFZ	C	5[B]	2	-	0/7/25/26	0/2/2/2
2	AF2	C	2[B]	2	-	0/3/25/26	0/3/3/3
2	GF2	C	1[C]	2	-	2/2/22/26	0/3/3/3
2	CFZ	C	3[B]	2	-	0/7/25/26	0/2/2/2
2	CFZ	C	5[C]	2	-	0/7/25/26	0/2/2/2
2	CFZ	C	12[A]	3,2	-	0/7/25/26	0/2/2/2
3	BRU	D	4[A]	3,2	-	0/7/21/22	0/2/2/2
2	AF2	C	2[C]	2	-	0/3/25/26	0/3/3/3
2	UFT	C	7[B]	2	-	1/7/25/26	0/2/2/2
2	CFZ	C	3[C]	2	-	0/7/25/26	0/2/2/2
2	GF2	C	8[A]	3,2	-	1/3/25/26	0/3/3/3
2	UFT	C	7[C]	2	-	2/7/25/26	0/2/2/2
3	BRU	D	4[B]	3	-	0/7/21/22	0/2/2/2
2	CFZ	C	12[B]	2	-	0/7/25/26	0/2/2/2
3	BRU	D	4[C]	3	-	0/7/21/22	0/2/2/2
2	CFZ	C	12[C]	2	-	0/7/25/26	0/2/2/2
2	GF2	C	8[B]	2	-	0/3/25/26	0/3/3/3
2	AF2	C	9[A]	3,2	-	0/3/25/26	0/3/3/3
2	GF2	C	8[C]	2	-	0/3/25/26	0/3/3/3

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11[B]	UFT	O5'-C5'	-7.33	1.26	1.44
2	C	6[C]	CFZ	O5'-C5'	-4.98	1.32	1.44
2	C	11[A]	UFT	O5'-C5'	-4.65	1.33	1.44
2	C	6[C]	CFZ	C2'-C3'	-4.45	1.46	1.52
2	C	12[C]	CFZ	C2'-C3'	-4.34	1.46	1.52
2	C	7[C]	UFT	C2-N1	4.20	1.45	1.38
2	C	2[C]	AF2	C2'-C1'	-3.92	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1[C]	GF2	O4'-C1'	3.79	1.46	1.41
2	C	9[A]	AF2	C2'-C3'	-3.71	1.47	1.52
2	C	4[B]	AF2	C2-N3	3.56	1.37	1.32
3	D	4[C]	BRU	C2-N1	3.54	1.44	1.38
2	C	10[A]	UFT	C2-N3	-3.53	1.31	1.38
2	C	10[B]	UFT	O2-C2	3.50	1.29	1.23
3	D	4[B]	BRU	C4-N3	-3.50	1.32	1.38
2	C	12[A]	CFZ	C2'-C1'	-3.47	1.48	1.53
2	C	10[B]	UFT	C5-C4	-3.44	1.36	1.43
2	C	7[C]	UFT	C4-N3	-3.44	1.32	1.38
3	D	4[B]	BRU	C6-N1	-3.37	1.32	1.38
2	C	10[C]	UFT	C2-N1	3.36	1.43	1.38
3	D	4[C]	BRU	C4-N3	-3.34	1.32	1.38
3	D	4[B]	BRU	O4-C4	3.32	1.29	1.23
2	C	8[A]	GF2	O4'-C1'	3.31	1.45	1.41
2	C	2[C]	AF2	C2'-C3'	-3.31	1.48	1.52
2	C	9[A]	AF2	C4-N3	-3.29	1.31	1.35
2	C	9[B]	AF2	F-C2'	-3.28	1.33	1.40
2	C	1[C]	GF2	C6-N1	-3.28	1.33	1.37
2	C	8[C]	GF2	C2'-C1'	-3.25	1.48	1.53
2	C	7[A]	UFT	O5'-C5'	-3.20	1.36	1.44
2	C	1[B]	GF2	C6-N1	-3.19	1.33	1.37
2	C	1[A]	GF2	C6-N1	-3.16	1.33	1.37
3	D	4[C]	BRU	C6-C5	3.13	1.40	1.34
2	C	5[A]	CFZ	C2'-C1'	-3.08	1.49	1.53
2	C	9[C]	AF2	C2-N3	3.06	1.37	1.32
2	C	5[B]	CFZ	C2'-C3'	-3.05	1.48	1.52
2	C	7[A]	UFT	C4-N3	-3.02	1.33	1.38
2	C	12[B]	CFZ	F2'-C2'	-3.01	1.33	1.40
3	D	4[B]	BRU	C2-N3	-3.01	1.32	1.38
3	D	4[A]	BRU	C4-N3	-2.95	1.33	1.38
3	D	4[A]	BRU	C6-N1	-2.93	1.33	1.38
3	D	4[C]	BRU	BR-C5	2.83	1.95	1.88
2	C	11[C]	UFT	C2-N3	-2.82	1.32	1.38
2	C	4[A]	AF2	C2'-C3'	-2.81	1.48	1.52
2	C	7[A]	UFT	C2'-C1'	-2.79	1.49	1.53
3	D	4[A]	BRU	C6-C5	2.78	1.39	1.34
2	C	8[C]	GF2	O6-C6	2.77	1.28	1.23
2	C	12[B]	CFZ	C2'-C1'	-2.73	1.49	1.53
2	C	7[A]	UFT	C2-N3	-2.73	1.33	1.38
2	C	12[A]	CFZ	C2'-C3'	-2.70	1.48	1.52
2	C	8[A]	GF2	C4-N3	-2.69	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	10[A]	UFT	O2-C2	2.67	1.27	1.23
2	C	10[B]	UFT	C2-N3	-2.65	1.33	1.38
2	C	7[B]	UFT	C4-N3	-2.62	1.33	1.38
2	C	11[C]	UFT	C4-N3	-2.61	1.33	1.38
2	C	10[B]	UFT	C2'-C3'	-2.60	1.49	1.52
2	C	6[B]	CFZ	C2'-C1'	-2.59	1.49	1.53
3	D	4[A]	BRU	BR-C5	-2.58	1.82	1.88
2	C	4[A]	AF2	C2-N3	2.56	1.36	1.32
2	C	9[A]	AF2	O5'-C5'	-2.56	1.38	1.44
2	C	5[A]	CFZ	C2'-C3'	-2.54	1.49	1.52
2	C	6[A]	CFZ	C2'-C1'	-2.51	1.49	1.53
2	C	4[C]	AF2	C2-N3	2.51	1.36	1.32
2	C	3[C]	CFZ	C2'-C3'	-2.49	1.49	1.52
2	C	9[A]	AF2	C2'-C1'	-2.48	1.49	1.53
3	D	4[A]	BRU	O4-C4	2.48	1.28	1.23
2	C	7[B]	UFT	C2-N3	-2.48	1.33	1.38
2	C	8[A]	GF2	C6-N1	-2.44	1.34	1.37
2	C	1[A]	GF2	O4'-C1'	2.44	1.44	1.41
2	C	7[B]	UFT	C6-N1	-2.41	1.32	1.38
2	C	2[B]	AF2	O4'-C1'	2.37	1.44	1.41
2	C	7[C]	UFT	C2'-C3'	-2.37	1.49	1.52
2	C	2[A]	AF2	C8-N7	2.36	1.38	1.34
2	C	8[B]	GF2	C6-N1	-2.35	1.34	1.37
2	C	6[B]	CFZ	O5'-C5'	-2.31	1.39	1.44
2	C	12[A]	CFZ	C2-N3	-2.31	1.31	1.36
2	C	3[C]	CFZ	C5-C4	-2.31	1.37	1.42
2	C	6[B]	CFZ	C2'-C3'	2.28	1.55	1.52
2	C	11[B]	UFT	C2'-C3'	2.26	1.55	1.52
2	C	9[B]	AF2	C2'-C3'	-2.25	1.49	1.52
2	C	9[C]	AF2	C2'-C3'	-2.25	1.49	1.52
2	C	7[B]	UFT	C5-C4	-2.24	1.38	1.43
2	C	2[B]	AF2	C2'-C1'	-2.21	1.50	1.53
2	C	8[A]	GF2	O6-C6	2.20	1.27	1.23
2	C	11[B]	UFT	C3'-C4'	-2.20	1.47	1.53
2	C	5[B]	CFZ	C3'-C4'	-2.19	1.47	1.53
2	C	7[A]	UFT	O3'-C3'	-2.19	1.37	1.43
2	C	8[C]	GF2	C4-N3	-2.18	1.32	1.37
2	C	8[A]	GF2	C2'-C3'	-2.18	1.49	1.52
2	C	3[B]	CFZ	C5-C4	-2.17	1.38	1.42
2	C	1[C]	GF2	C2'-C1'	-2.17	1.50	1.53
2	C	2[A]	AF2	O5'-C5'	-2.16	1.39	1.44
2	C	7[C]	UFT	C2-N3	-2.16	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3[B]	CFZ	C2'-C1'	-2.12	1.50	1.53
2	C	10[C]	UFT	C2'-C3'	-2.12	1.49	1.52
2	C	6[A]	CFZ	O5'-C5'	-2.11	1.39	1.44
2	C	10[C]	UFT	C6-C5	2.11	1.39	1.35
2	C	1[A]	GF2	C2'-C3'	-2.11	1.49	1.52
2	C	12[C]	CFZ	C6-C5	2.09	1.39	1.35
2	C	3[C]	CFZ	C2-N3	-2.08	1.32	1.36
2	C	6[B]	CFZ	O3'-C3'	2.07	1.47	1.43
2	C	6[B]	CFZ	C4-N4	2.07	1.38	1.33
2	C	1[C]	GF2	F-C2'	-2.06	1.35	1.40
2	C	3[A]	CFZ	C2'-C3'	-2.06	1.49	1.52
2	C	5[A]	CFZ	O4'-C1'	2.06	1.46	1.42
2	C	2[C]	AF2	C2-N3	2.05	1.35	1.32
2	C	3[B]	CFZ	C2'-C3'	-2.04	1.49	1.52
2	C	10[A]	UFT	C5-C4	-2.04	1.39	1.43
2	C	11[C]	UFT	C2'-C1'	-2.04	1.50	1.53
2	C	12[C]	CFZ	O5'-C5'	-2.04	1.39	1.44
2	C	7[B]	UFT	O2-C2	2.04	1.26	1.23
2	C	12[B]	CFZ	O5'-C5'	-2.03	1.39	1.44
2	C	3[A]	CFZ	C6-C5	2.03	1.39	1.35
2	C	10[A]	UFT	O5'-C5'	-2.02	1.39	1.44
2	C	11[C]	UFT	C2-N1	2.02	1.41	1.38
3	D	4[C]	BRU	C4-C5	2.01	1.49	1.45
2	C	9[B]	AF2	C4-N3	-2.01	1.32	1.35
2	C	11[B]	UFT	C5-C4	-2.01	1.39	1.43
2	C	8[C]	GF2	C2'-C3'	-2.00	1.49	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4[C]	BRU	C5-C4-N3	6.02	120.27	113.34
2	C	11[A]	UFT	O2-C2-N1	-5.50	115.47	122.79
2	C	11[B]	UFT	C4-N3-C2	-5.15	119.79	126.58
2	C	6[B]	CFZ	C2'-C3'-C4'	-5.12	95.78	102.40
2	C	10[C]	UFT	C4-N3-C2	-5.02	119.96	126.58
2	C	7[B]	UFT	C4-N3-C2	-4.97	120.02	126.58
2	C	9[A]	AF2	C2'-C3'-C4'	-4.89	96.09	102.40
2	C	11[A]	UFT	C4-N3-C2	-4.77	120.29	126.58
2	C	11[C]	UFT	C4-N3-C2	-4.67	120.42	126.58
2	C	9[C]	AF2	N3-C2-N1	-4.64	121.43	128.68
3	D	4[C]	BRU	N3-C2-N1	4.63	121.04	114.89
2	C	4[B]	AF2	N3-C2-N1	-4.60	121.49	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4[C]	BRU	C4-N3-C2	-4.56	121.45	127.35
3	D	4[B]	BRU	N3-C2-N1	4.47	120.82	114.89
2	C	11[B]	UFT	O2-C2-N1	-4.43	116.90	122.79
2	C	10[B]	UFT	C4-N3-C2	-4.38	120.80	126.58
2	C	7[C]	UFT	C4-N3-C2	-4.36	120.83	126.58
2	C	5[A]	CFZ	C2'-C3'-C4'	-4.27	96.89	102.40
3	D	4[C]	BRU	O4-C4-C5	-4.26	120.50	125.84
2	C	10[A]	UFT	C4-N3-C2	-4.23	121.00	126.58
2	C	7[C]	UFT	N3-C2-N1	4.19	120.45	114.89
2	C	7[B]	UFT	O4-C4-C5	-4.13	117.89	125.16
2	C	7[A]	UFT	C4-N3-C2	-4.13	121.14	126.58
2	C	9[A]	AF2	N3-C2-N1	-4.07	122.31	128.68
2	C	11[C]	UFT	N3-C2-N1	4.07	120.30	114.89
2	C	11[A]	UFT	N3-C2-N1	4.07	120.29	114.89
2	C	11[C]	UFT	C5-C4-N3	4.00	120.82	114.84
2	C	4[C]	AF2	N3-C2-N1	-3.94	122.52	128.68
2	C	5[B]	CFZ	C2'-C1'-N1	-3.94	108.17	114.20
2	C	10[B]	UFT	C5-C4-N3	3.93	120.72	114.84
2	C	9[B]	AF2	N3-C2-N1	-3.91	122.56	128.68
2	C	7[B]	UFT	C5-C4-N3	3.90	120.67	114.84
2	C	2[B]	AF2	N3-C2-N1	-3.88	122.61	128.68
2	C	10[C]	UFT	C5-C4-N3	3.84	120.59	114.84
2	C	2[A]	AF2	N3-C2-N1	-3.84	122.68	128.68
3	D	4[B]	BRU	C4-N3-C2	-3.83	122.40	127.35
2	C	5[A]	CFZ	C2'-C1'-N1	-3.82	108.36	114.20
2	C	10[C]	UFT	N3-C2-N1	3.80	119.94	114.89
2	C	10[B]	UFT	O4-C4-C5	-3.74	118.57	125.16
2	C	7[A]	UFT	C5-C4-N3	3.72	120.41	114.84
3	D	4[A]	BRU	N3-C2-N1	3.66	119.75	114.89
3	D	4[A]	BRU	O4-C4-C5	-3.64	121.27	125.84
2	C	7[A]	UFT	N3-C2-N1	3.64	119.72	114.89
2	C	4[A]	AF2	N3-C2-N1	-3.62	123.01	128.68
2	C	2[C]	AF2	N3-C2-N1	-3.55	123.13	128.68
2	C	11[B]	UFT	C5-C4-N3	3.53	120.13	114.84
2	C	10[A]	UFT	N3-C2-N1	3.52	119.56	114.89
2	C	7[C]	UFT	C5-C4-N3	3.44	119.99	114.84
2	C	5[C]	CFZ	C2'-C1'-N1	-3.41	109.00	114.20
2	C	10[A]	UFT	C5-C4-N3	3.40	119.92	114.84
3	D	4[C]	BRU	C6-C5-C4	-3.35	117.28	120.67
2	C	12[B]	CFZ	C2'-C3'-C4'	-3.34	98.09	102.40
2	C	6[A]	CFZ	C2'-C3'-C4'	-3.32	98.11	102.40
2	C	10[A]	UFT	O4-C4-C5	-3.27	119.41	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7[C]	UFT	C1'-N1-C2	3.23	123.42	117.57
2	C	11[B]	UFT	O4-C4-C5	-3.22	119.49	125.16
2	C	10[B]	UFT	N3-C2-N1	3.20	119.14	114.89
3	D	4[A]	BRU	C5-C4-N3	3.17	116.99	113.34
3	D	4[B]	BRU	C5-C4-N3	3.13	116.94	113.34
3	D	4[A]	BRU	C4-N3-C2	-3.11	123.33	127.35
2	C	7[B]	UFT	N3-C2-N1	3.09	118.99	114.89
2	C	12[C]	CFZ	C2'-C3'-C4'	-3.07	98.43	102.40
2	C	11[B]	UFT	N3-C2-N1	3.07	118.97	114.89
2	C	10[C]	UFT	O4-C4-C5	-3.05	119.79	125.16
2	C	6[A]	CFZ	C3'-C2'-C1'	-3.03	99.46	103.13
3	D	4[B]	BRU	O4-C4-C5	-3.01	122.06	125.84
2	C	11[A]	UFT	C5-C4-N3	3.01	119.34	114.84
2	C	3[C]	CFZ	C2'-C1'-N1	-3.00	109.62	114.20
3	D	4[B]	BRU	BR-C5-C4	2.99	121.51	118.03
2	C	10[A]	UFT	C3'-C2'-C1'	-2.96	99.54	103.13
2	C	2[B]	AF2	C4-C5-N7	-2.95	106.33	109.40
2	C	7[A]	UFT	O4-C4-C5	-2.94	120.00	125.16
2	C	6[B]	CFZ	O3'-C3'-C2'	2.92	122.50	111.57
2	C	6[C]	CFZ	C2'-C1'-N1	-2.91	109.75	114.20
2	C	9[A]	AF2	C1'-N9-C4	-2.91	121.52	126.64
2	C	11[C]	UFT	O4-C4-C5	-2.91	120.04	125.16
2	C	11[C]	UFT	F2'-C2'-C3'	2.88	115.25	109.22
2	C	7[C]	UFT	O2-C2-N3	-2.88	116.14	121.50
3	D	4[B]	BRU	C2'-C1'-N1	-2.87	107.15	113.77
2	C	11[C]	UFT	C2'-C1'-N1	-2.84	109.86	114.20
2	C	10[B]	UFT	O2-C2-N1	-2.83	119.02	122.79
2	C	6[C]	CFZ	O4'-C4'-C3'	2.76	110.57	105.11
2	C	1[A]	GF2	C5-C6-N1	2.73	118.77	113.95
2	C	3[A]	CFZ	C2'-C3'-C4'	-2.70	98.92	102.40
2	C	9[B]	AF2	C2'-C3'-C4'	-2.70	98.92	102.40
2	C	2[C]	AF2	C4-C5-N7	-2.70	106.59	109.40
2	C	7[C]	UFT	C6-N1-C2	-2.66	117.59	120.99
2	C	2[A]	AF2	C2-N1-C6	2.64	123.26	118.75
2	C	7[B]	UFT	O2-C2-N1	-2.61	119.32	122.79
3	D	4[B]	BRU	O4'-C1'-N1	2.61	112.52	107.86
2	C	1[B]	GF2	C5-C6-N1	2.60	118.54	113.95
2	C	10[C]	UFT	C2'-C1'-N1	-2.58	110.26	114.20
2	C	1[C]	GF2	C8-N7-C5	2.57	107.89	102.99
2	C	10[A]	UFT	O2-C2-N1	-2.55	119.40	122.79
2	C	5[A]	CFZ	O4'-C1'-N1	2.51	114.11	108.36
2	C	2[B]	AF2	C2'-C3'-C4'	-2.49	99.18	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8[C]	GF2	C8-N7-C5	2.47	107.70	102.99
2	C	10[B]	UFT	C2'-C1'-N1	-2.47	110.43	114.20
3	D	4[B]	BRU	BR-C5-C6	-2.47	117.19	120.64
2	C	2[C]	AF2	C2'-C3'-C4'	-2.46	99.22	102.40
2	C	6[B]	CFZ	F2'-C2'-C3'	2.45	114.34	109.22
2	C	11[B]	UFT	O3'-C3'-C2'	2.44	120.70	111.57
3	D	4[A]	BRU	O2-C2-N1	-2.42	119.57	122.79
2	C	4[A]	AF2	C5-C6-N6	2.42	124.03	120.35
2	C	4[C]	AF2	C4-C5-N7	-2.41	106.88	109.40
2	C	7[C]	UFT	O4-C4-C5	-2.41	120.93	125.16
2	C	5[A]	CFZ	O4'-C4'-C5'	2.41	117.29	109.37
3	D	4[B]	BRU	O2-C2-N1	-2.40	119.60	122.79
2	C	4[B]	AF2	C1'-N9-C4	-2.39	122.45	126.64
2	C	9[B]	AF2	C1'-N9-C4	-2.39	122.45	126.64
2	C	10[B]	UFT	C3'-C2'-C1'	-2.38	100.25	103.13
2	C	12[B]	CFZ	C3'-C2'-C1'	2.37	105.99	103.13
2	C	1[B]	GF2	F-C2'-C1'	-2.36	104.15	109.08
2	C	11[C]	UFT	F2'-C2'-C1'	-2.36	104.16	109.08
2	C	9[B]	AF2	C4-C5-N7	-2.35	106.95	109.40
2	C	1[C]	GF2	O4'-C4'-C5'	2.32	114.23	109.21
2	C	6[C]	CFZ	O5'-C5'-C4'	-2.32	101.12	108.99
2	C	12[A]	CFZ	C5-C6-N1	-2.31	117.93	121.81
2	C	8[A]	GF2	C8-N7-C5	2.31	107.39	102.99
2	C	11[A]	UFT	O4-C4-C5	-2.31	121.10	125.16
2	C	6[B]	CFZ	C2'-C1'-N1	-2.30	110.68	114.20
2	C	1[C]	GF2	C5-C6-N1	2.30	118.02	113.95
2	C	7[A]	UFT	O2-C2-N1	-2.29	119.74	122.79
3	D	4[C]	BRU	BR-C5-C4	2.29	120.69	118.03
2	C	8[A]	GF2	C2-N1-C6	-2.29	120.89	125.10
2	C	11[C]	UFT	C2'-C3'-C4'	-2.26	99.48	102.40
2	C	6[A]	CFZ	O3'-C3'-C2'	2.25	119.97	111.57
2	C	8[C]	GF2	C2-N1-C6	-2.23	120.98	125.10
2	C	7[C]	UFT	C2'-C1'-N1	-2.21	110.82	114.20
2	C	7[B]	UFT	F2'-C2'-C3'	2.19	113.81	109.22
2	C	7[A]	UFT	F2'-C2'-C3'	2.18	113.78	109.22
2	C	6[A]	CFZ	C5-C6-N1	-2.17	118.18	121.81
2	C	8[C]	GF2	O6-C6-C5	-2.16	120.14	124.37
2	C	4[A]	AF2	C2-N1-C6	2.16	122.44	118.75
2	C	4[B]	AF2	C2-N1-C6	2.16	122.44	118.75
2	C	2[A]	AF2	C4-C5-N7	-2.15	107.16	109.40
2	C	12[C]	CFZ	C2'-C1'-N1	-2.14	110.93	114.20
2	C	11[B]	UFT	C2'-C3'-C4'	-2.13	99.65	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4[A]	BRU	BR-C5-C4	2.10	120.47	118.03
2	C	12[A]	CFZ	O2-C2-N3	-2.09	118.93	122.33
2	C	7[B]	UFT	C2'-C3'-C4'	2.08	105.09	102.40
3	D	4[C]	BRU	O3'-C3'-C4'	-2.08	102.15	110.10
2	C	11[C]	UFT	O4'-C1'-N1	2.08	113.11	108.36
2	C	9[A]	AF2	C4-C5-N7	-2.07	107.24	109.40
2	C	1[B]	GF2	C3'-C2'-C1'	2.06	105.63	103.13
2	C	12[C]	CFZ	F2'-C2'-C3'	-2.06	104.91	109.22
3	D	4[C]	BRU	O2-C2-N3	-2.05	117.69	121.50
2	C	8[C]	GF2	O6-C6-N1	2.04	123.06	120.65
2	C	2[A]	AF2	C1'-N9-C4	-2.04	123.06	126.64
3	D	4[C]	BRU	C6-N1-C2	-2.03	119.24	121.30
2	C	4[B]	AF2	C3'-C2'-C1'	-2.03	100.67	103.13

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6[C]	CFZ	C3'-C4'-C5'-O5'
2	C	7[C]	UFT	O4'-C4'-C5'-O5'
2	C	11[A]	UFT	O4'-C4'-C5'-O5'
2	C	11[A]	UFT	C3'-C4'-C5'-O5'
2	C	11[B]	UFT	O4'-C4'-C5'-O5'
2	C	11[B]	UFT	C3'-C4'-C5'-O5'
2	C	5[A]	CFZ	C3'-C4'-C5'-O5'
2	C	5[A]	CFZ	O4'-C4'-C5'-O5'
2	C	7[C]	UFT	C3'-C4'-C5'-O5'
2	C	1[C]	GF2	O4'-C4'-C5'-O5'
2	C	6[C]	CFZ	O4'-C4'-C5'-O5'
2	C	1[C]	GF2	C3'-C4'-C5'-O5'
2	C	8[A]	GF2	O4'-C4'-C5'-O5'
2	C	7[A]	UFT	C3'-C4'-C5'-O5'
2	C	7[B]	UFT	C3'-C4'-C5'-O5'
2	C	10[C]	UFT	C3'-C4'-C5'-O5'
2	C	9[B]	AF2	O4'-C4'-C5'-O5'
2	C	10[C]	UFT	O4'-C4'-C5'-O5'
2	C	9[B]	AF2	C3'-C4'-C5'-O5'

There are no ring outliers.

23 monomers are involved in 63 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10[A]	UFT	1	0
2	C	9[B]	AF2	2	0
2	C	9[C]	AF2	1	0
2	C	10[B]	UFT	1	0
2	C	11[B]	UFT	2	0
2	C	10[C]	UFT	4	0
2	C	11[C]	UFT	4	0
2	C	6[C]	CFZ	15	0
2	C	5[A]	CFZ	1	0
2	C	4[C]	AF2	9	0
2	C	2[B]	AF2	1	0
2	C	3[B]	CFZ	1	0
2	C	5[C]	CFZ	6	0
2	C	2[C]	AF2	1	0
2	C	7[B]	UFT	1	0
2	C	3[C]	CFZ	4	0
2	C	7[C]	UFT	13	0
2	C	12[B]	CFZ	2	0
3	D	4[C]	BRU	4	0
2	C	12[C]	CFZ	9	0
2	C	8[B]	GF2	1	0
2	C	9[A]	AF2	1	0
2	C	8[C]	GF2	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
6	PEG	A	203	-	6,6,6	0.80	0	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	D	101	-	5,5,5	0.92	0	5,5,5	0.84	0

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
6	PEG	A	203	-	-	3/4/4/4	-
7	GOL	D	101	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	101	GOL	C1-C2-C3-O3
6	A	203	PEG	O2-C3-C4-O4
7	D	101	GOL	O2-C2-C3-O3
6	A	203	PEG	C1-C2-O2-C3
6	A	203	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	203	PEG	6	0
7	D	101	GOL	2	0

## 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, 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	131/142 (92%)	0.59	5 (3%) 40 44	8, 17, 28, 40	0
1	B	133/142 (93%)	0.54	1 (0%) 86 89	8, 16, 30, 41	0
2	C	0/12	-	-	-	-
3	D	11/12 (91%)	0.56	0 100 100	12, 14, 18, 19	0
All	All	275/308 (89%)	0.56	6 (2%) 62 67	8, 16, 28, 41	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	THR	2.9
1	A	74	SER	2.9
1	A	89	LYS	2.6
1	A	154	GLU	2.4
1	A	193	TYR	2.3
1	B	184	ASP	2.3

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	UFT	C	7[A]	20/21	0.90	0.17	14,17,18,19	20
2	UFT	C	7[B]	20/21	0.90	0.17	16,18,24,24	20
2	UFT	C	7[C]	20/21	0.90	0.17	13,13,15,16	20
2	GF2	C	1[A]	20/24	0.91	0.17	11,12,14,17	20
2	GF2	C	1[B]	20/24	0.91	0.17	14,16,19,19	20
2	GF2	C	1[C]	20/24	0.91	0.17	13,13,14,14	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CFZ	C	3[A]	20/21	0.93	0.13	12,14,20,20	20
2	CFZ	C	3[B]	20/21	0.93	0.13	15,18,23,24	20
2	CFZ	C	3[C]	20/21	0.93	0.13	9,10,11,11	20
2	AF2	C	2[A]	22/23	0.93	0.13	13,14,15,16	22
2	AF2	C	2[B]	22/23	0.93	0.13	15,19,21,22	22
2	AF2	C	2[C]	22/23	0.93	0.13	10,11,13,14	22
2	GF2	C	8[A]	23/24	0.93	0.13	11,13,18,19	23
2	GF2	C	8[B]	23/24	0.93	0.13	14,16,19,21	23
2	GF2	C	8[C]	23/24	0.93	0.13	11,12,13,14	23
2	CFZ	C	6[A]	20/21	0.94	0.12	11,12,13,15	20
2	CFZ	C	6[B]	20/21	0.94	0.12	11,12,13,16	20
2	CFZ	C	6[C]	20/21	0.94	0.12	11,12,13,14	20
2	AF2	C	9[A]	22/23	0.94	0.14	11,12,20,22	22
2	AF2	C	9[B]	22/23	0.94	0.14	13,14,22,24	22
2	AF2	C	9[C]	22/23	0.94	0.14	10,10,12,12	22
2	CFZ	C	12[A]	20/21	0.94	0.14	10,11,12,12	20
2	CFZ	C	12[B]	20/21	0.94	0.14	11,12,13,13	20
2	CFZ	C	12[C]	20/21	0.94	0.14	14,15,16,16	20
3	BRU	D	4[A]	20/21	0.94	0.12	8,11,12,15	20
3	BRU	D	4[B]	20/21	0.94	0.12	11,14,18,20	20
3	BRU	D	4[C]	20/21	0.94	0.12	10,12,17,28	20
2	UFT	C	10[A]	20/21	0.95	0.12	9,9,12,12	20
2	UFT	C	10[B]	20/21	0.95	0.12	11,12,14,17	20
2	UFT	C	10[C]	20/21	0.95	0.12	10,10,11,11	20
2	AF2	C	4[A]	22/23	0.95	0.14	9,11,15,19	22
2	AF2	C	4[B]	22/23	0.95	0.14	15,17,19,21	22
2	AF2	C	4[C]	22/23	0.95	0.14	9,12,16,17	22
2	CFZ	C	5[A]	20/21	0.95	0.11	9,11,13,13	20
2	CFZ	C	5[B]	20/21	0.95	0.11	12,13,15,15	20
2	CFZ	C	5[C]	20/21	0.95	0.11	9,10,11,11	20
2	UFT	C	11[A]	20/21	0.96	0.11	11,11,12,12	20
2	UFT	C	11[B]	20/21	0.96	0.11	9,11,12,13	20
2	UFT	C	11[C]	20/21	0.96	0.11	11,12,12,13	20

### 6.3 Carbohydrates

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	D	101	6/6	0.83	0.16	22,28,33,35	0
6	PEG	A	203	7/7	0.91	0.17	13,18,32,34	0
4	NA	A	201	1/1	0.94	0.09	21,21,21,21	0
5	CL	A	202	1/1	0.98	0.05	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.