



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 08:52 PM EDT

PDB ID : 5B2P
Title : Crystal structure of Francisella novicida Cas9 in complex with sgRNA and target DNA (TGA PAM)
Authors : Hirano, H.; Nishimasu, H.; Nakane, T.; Ishitani, R.; Nureki, O.
Deposited on : 2016-02-01
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

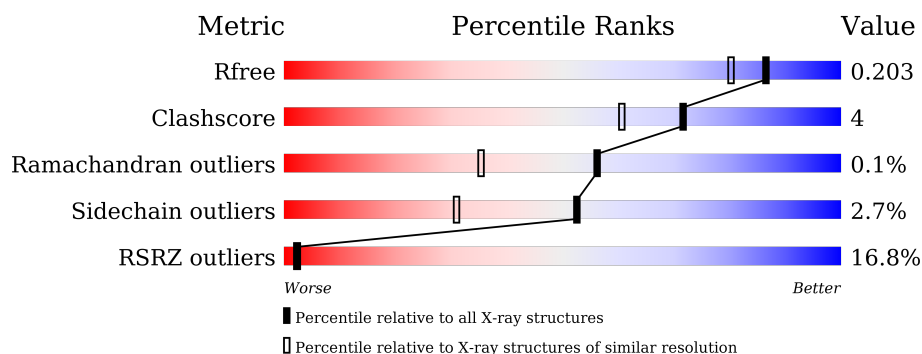
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	1632	<div> <div>16%</div> <div> <div>79%</div> <div>9%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	94	<div> <div>27%</div> <div>62%</div> <div>12%</div> </div>
3	C	30	<div> <div>7%</div> <div>47%</div> <div>43%</div> <div>10%</div> </div>
4	D	9	<div> <div>33%</div> <div>67%</div> <div>22%</div> <div>11%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ACT	B	120	-	-	-	X
9	EDO	A	1724	-	-	-	X
9	EDO	A	1726	-	-	-	X
9	EDO	B	110	-	-	-	X
9	EDO	B	114	-	-	-	X
9	EDO	B	115	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15757 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 CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1455	Total	C	N	O	S	0	18	0
			11809	7555	2030	2193	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0Q5Y3
A	-1	SER	-	expression tag	UNP A0Q5Y3
A	0	HIS	-	expression tag	UNP A0Q5Y3
A	995	ALA	ASN	engineered mutation	UNP A0Q5Y3

- Molecule 2 is DNA/RNA hybrid called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	P	0	0	0
			1991	886	350	661	94			

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			596	286	104	177	29			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*GP*AP*TP*AP*TP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	P	0	0	0
			184	89	34	53	8			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Na 2 2	0	0
6	A	2	Total Na 2 2	0	0

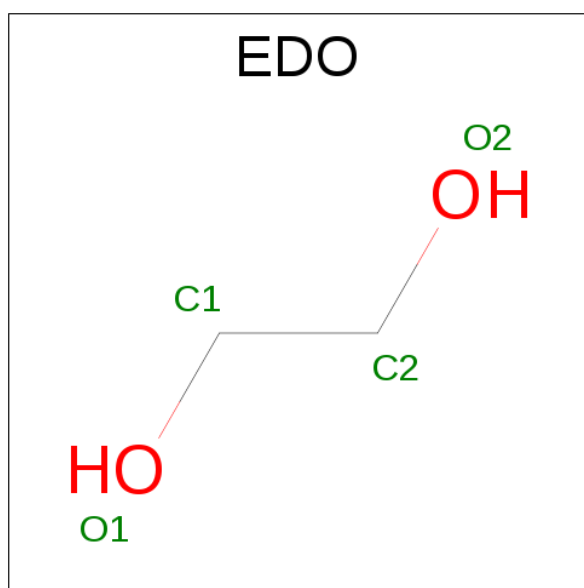
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	6	Total Ca 6 6	0	0
8	A	11	Total Ca 11 11	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



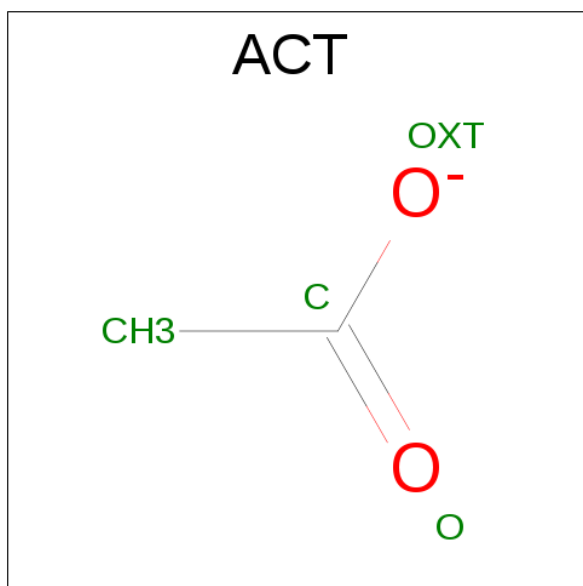
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

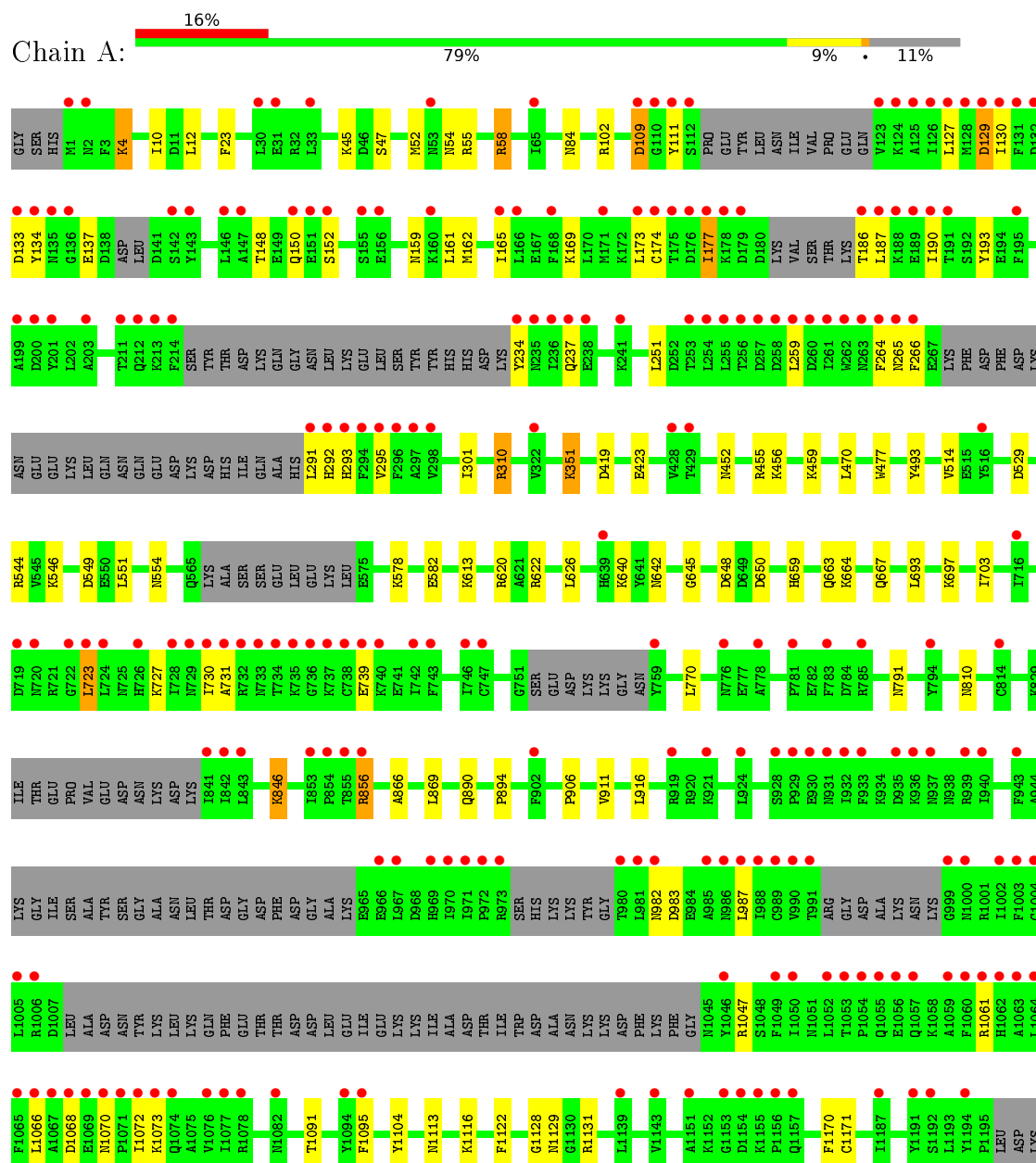
- Molecule 11 is water.

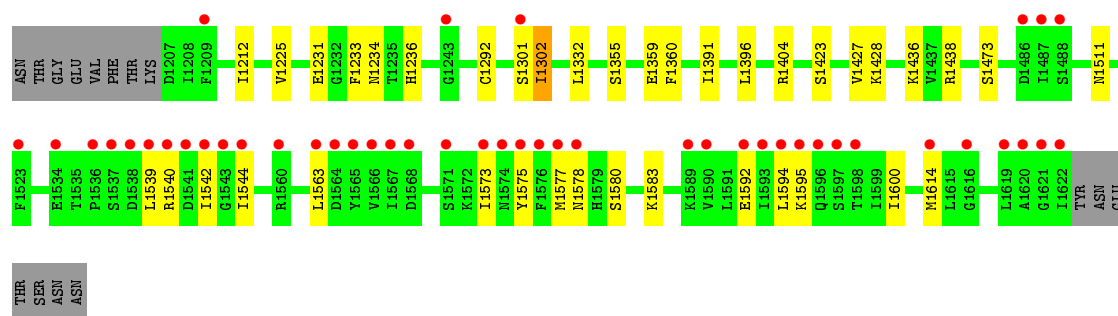
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	639	Total	O	0	0
			639	639		
11	B	342	Total	O	0	0
			342	342		
11	C	68	Total	O	0	0
			68	68		
11	D	4	Total	O	0	0
			4	4		

3 Residue-property plots

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

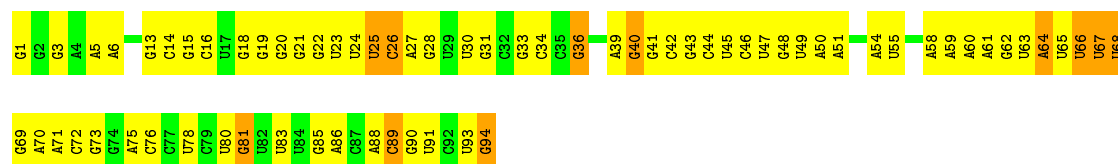
- Molecule 1: CRISPR-associated endonuclease Cas9





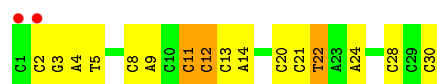
• Molecule 2: Guide RNA

Chain B: 27% 62% 12%



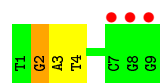
• Molecule 3: Target DNA

Chain C: 7% 47% 43% 10%



• Molecule 4: DNA (5'-D(*TP*GP*AP*TP*AP*TP*CP*GP*G)-3')

Chain D: 33% 67% 22% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 159.27Å 96.67Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	46.26 – 1.70 46.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.26-1.70) 98.8 (46.26-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.180 , 0.203 0.179 , 0.203	Depositor DCC
R_{free} test set	12758 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 255174 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, NA, CA, EDO, ACT

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	0.66	2/12080 (0.0%)	0.73	11/16292 (0.1%)
2	B	1.61	30/2224 (1.3%)	1.98	122/3465 (3.5%)
3	C	1.62	10/665 (1.5%)	1.55	10/1020 (1.0%)
4	D	1.24	0/206	1.11	1/317 (0.3%)
All	All	0.93	42/15175 (0.3%)	1.09	144/21094 (0.7%)

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
2	B	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9	DA	N3-C4	-9.14	1.29	1.34
2	B	43	G	N7-C5	9.11	1.44	1.39
2	B	46	C	N1-C6	8.56	1.42	1.37
2	B	76	C	N1-C6	7.11	1.41	1.37
3	C	20	DC	N3-C4	-6.90	1.29	1.33
3	C	22	DT	C3'-O3'	-6.88	1.35	1.44
2	B	33	G	N7-C5	6.68	1.43	1.39
2	B	19	G	C2-N3	6.64	1.38	1.32
2	B	69	G	C6-N1	6.55	1.44	1.39
2	B	45	U	C4-O4	6.32	1.28	1.23
3	C	9	DA	C6-N1	-6.30	1.31	1.35
2	B	31	G	C6-N1	6.08	1.43	1.39
2	B	25	U	C4-O4	5.89	1.28	1.23
2	B	60	A	C6-N1	-5.82	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	48	G	C2-N3	5.76	1.37	1.32
2	B	20	G	C2-N2	5.76	1.40	1.34
2	B	15	G	C8-N7	5.67	1.34	1.30
2	B	6	A	N7-C5	5.58	1.42	1.39
3	C	8	DC	C4-C5	5.50	1.47	1.43
2	B	71	A	N3-C4	5.45	1.38	1.34
2	B	62	G	C8-N7	5.44	1.34	1.30
2	B	21	G	C2-N2	5.43	1.40	1.34
3	C	20	DC	C4'-O4'	5.41	1.50	1.45
2	B	80	U	N1-C6	5.36	1.42	1.38
2	B	81	G	C8-N7	5.35	1.34	1.30
2	B	23	U	C4-C5	5.35	1.48	1.43
2	B	28	G	C2-N3	5.32	1.37	1.32
2	B	22	G	C2-N2	5.28	1.39	1.34
2	B	71	A	N7-C5	5.28	1.42	1.39
2	B	18	G	N1-C2	-5.26	1.33	1.37
2	B	26	C	C4-N4	5.25	1.38	1.33
2	B	94	G	N7-C5	5.21	1.42	1.39
3	C	14	DA	N3-C4	-5.21	1.31	1.34
2	B	51	A	N7-C5	-5.20	1.36	1.39
2	B	60	A	N9-C4	5.16	1.41	1.37
3	C	9	DA	C8-N7	5.15	1.35	1.31
3	C	28	DC	C4'-O4'	-5.14	1.40	1.45
2	B	60	A	N3-C4	-5.12	1.31	1.34
1	A	310	ARG	CG-CD	5.12	1.64	1.51
3	C	13	DC	C2-N3	-5.10	1.31	1.35
2	B	28	G	N3-C4	5.05	1.39	1.35
1	A	1355	SER	CB-OG	5.00	1.48	1.42

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	DC	O5'-P-OP2	-12.73	94.24	105.70
2	B	24	U	C5-C6-N1	-11.26	117.07	122.70
2	B	27	A	O5'-P-OP2	-10.63	96.13	105.70
3	C	11	DC	O5'-P-OP2	-9.59	97.07	105.70
2	B	68	U	C4-C5-C6	9.31	125.29	119.70
2	B	93	U	N3-C2-O2	8.97	128.48	122.20
2	B	25	U	N3-C4-C5	8.86	119.91	114.60
2	B	72	C	N3-C4-C5	8.72	125.39	121.90
1	A	58[A]	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	58[B]	ARG	NE-CZ-NH1	8.70	124.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	C	C4-C5-C6	-8.68	113.06	117.40
2	B	25	U	C6-N1-C2	8.51	126.11	121.00
3	C	11	DC	O4'-C4'-C3'	-8.43	100.94	106.00
2	B	47	U	C2-N3-C4	-8.05	122.17	127.00
2	B	70	A	N1-C2-N3	-8.02	125.29	129.30
2	B	21	G	C4-C5-N7	7.95	113.98	110.80
3	C	9	DA	O5'-P-OP2	-7.85	98.63	105.70
2	B	66	U	O5'-P-OP1	-7.66	98.81	105.70
2	B	20	G	N1-C2-N2	7.61	123.05	116.20
1	A	310	ARG	CG-CD-NE	-7.57	95.91	111.80
2	B	46	C	C2-N3-C4	7.57	123.68	119.90
3	C	11	DC	OP2-P-O3'	7.53	121.76	105.20
2	B	70	A	C4-C5-C6	-7.50	113.25	117.00
2	B	81	G	N3-C4-N9	-7.40	121.56	126.00
2	B	47	U	C5-C6-N1	-7.40	119.00	122.70
2	B	51	A	C6-N1-C2	7.38	123.03	118.60
2	B	72	C	C6-N1-C2	7.32	123.23	120.30
2	B	91	U	N3-C2-O2	7.32	127.32	122.20
2	B	63	U	C5-C6-N1	-7.30	119.05	122.70
2	B	25	U	C2-N3-C4	-7.16	122.70	127.00
2	B	21	G	C5-N7-C8	-7.16	100.72	104.30
2	B	25	U	C5-C4-O4	-7.10	121.64	125.90
2	B	27	A	N1-C6-N6	7.07	122.84	118.60
2	B	68	U	C5-C6-N1	-7.04	119.18	122.70
4	D	2	DG	O4'-C1'-N9	-6.96	103.13	108.00
2	B	67	U	N1-C2-N3	6.90	119.04	114.90
2	B	70	A	C6-C5-N7	6.85	137.09	132.30
3	C	22	DT	O5'-P-OP1	-6.84	99.54	105.70
2	B	83	U	O5'-P-OP1	-6.83	99.56	105.70
2	B	13	G	C5-C6-O6	-6.82	124.51	128.60
2	B	19	G	N1-C2-N2	6.80	122.32	116.20
2	B	23	U	C5-C4-O4	-6.79	121.83	125.90
2	B	66	U	O5'-P-OP2	6.72	118.76	110.70
2	B	86	A	O4'-C1'-N9	6.72	113.58	108.20
2	B	81	G	C6-N1-C2	6.68	129.11	125.10
3	C	11	DC	OP1-P-OP2	6.66	129.60	119.60
1	A	310	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	B	25	U	C5-C6-N1	-6.64	119.38	122.70
2	B	21	G	N3-C4-C5	6.64	131.92	128.60
2	B	42	C	N3-C2-O2	6.62	126.54	121.90
2	B	85	G	N1-C6-O6	-6.53	115.98	119.90
2	B	20	G	N3-C2-N2	-6.53	115.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	G	N1-C6-O6	6.52	123.81	119.90
2	B	81	G	C5-C6-N1	-6.52	108.24	111.50
2	B	75	A	C2-N3-C4	-6.48	107.36	110.60
2	B	30	U	N3-C2-O2	6.46	126.72	122.20
2	B	55	U	C4-C5-C6	-6.44	115.83	119.70
2	B	67	U	C6-N1-C2	-6.43	117.14	121.00
2	B	67	U	O5'-P-OP2	6.43	118.41	110.70
2	B	3	G	C5-C6-O6	-6.41	124.75	128.60
2	B	64	A	N7-C8-N9	-6.38	110.61	113.80
2	B	19	G	N3-C2-N2	-6.37	115.44	119.90
2	B	24	U	C6-N1-C2	6.36	124.82	121.00
2	B	68	U	N1-C2-N3	6.34	118.71	114.90
2	B	88	A	N1-C6-N6	6.33	122.39	118.60
2	B	55	U	N3-C4-C5	6.30	118.38	114.60
2	B	69	G	C5-C6-N1	6.24	114.62	111.50
2	B	58	A	O5'-P-OP1	-6.21	100.11	105.70
2	B	81	G	C2-N3-C4	-6.18	108.81	111.90
2	B	60	A	N1-C2-N3	-6.16	126.22	129.30
2	B	31	G	O5'-P-OP2	-6.16	100.16	105.70
2	B	67	U	OP1-P-OP2	-6.12	110.42	119.60
2	B	41	G	C2-N3-C4	6.11	114.96	111.90
2	B	26	C	C5-C6-N1	6.09	124.05	121.00
2	B	62	G	N1-C6-O6	-6.09	116.24	119.90
2	B	34	C	N3-C4-C5	-6.08	119.47	121.90
2	B	89	C	N3-C4-C5	6.08	124.33	121.90
2	B	88	A	C5-C6-N1	-6.06	114.67	117.70
2	B	34	C	O5'-P-OP1	-6.03	100.28	105.70
2	B	61	A	C5-C6-N1	-6.02	114.69	117.70
2	B	27	A	C2-N3-C4	-5.99	107.61	110.60
2	B	34	C	C5'-C4'-C3'	-5.99	106.42	116.00
2	B	78	U	C5-C6-N1	-5.99	119.71	122.70
2	B	81	G	N3-C4-C5	5.93	131.57	128.60
2	B	61	A	C6-N1-C2	5.91	122.15	118.60
2	B	61	A	N3-C4-N9	-5.90	122.68	127.40
2	B	44	C	O5'-P-OP2	-5.88	100.41	105.70
2	B	21	G	N1-C2-N2	5.87	121.48	116.20
1	A	55	ARG	NE-CZ-NH1	-5.86	117.37	120.30
3	C	22	DT	N3-C4-O4	5.86	123.42	119.90
2	B	67	U	N3-C2-O2	-5.86	118.10	122.20
2	B	90	G	C5-C6-O6	-5.86	125.08	128.60
2	B	40	G	OP2-P-O3'	5.85	118.06	105.20
2	B	42	C	N3-C4-C5	5.84	124.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	A	C5-C6-N1	5.79	120.59	117.70
2	B	91	U	N1-C2-O2	-5.78	118.75	122.80
2	B	54	A	N7-C8-N9	-5.71	110.94	113.80
2	B	65	U	C2-N3-C4	-5.70	123.58	127.00
2	B	60	A	C2-N3-C4	5.63	113.42	110.60
2	B	34	C	C2-N3-C4	5.60	122.70	119.90
2	B	66	U	OP1-P-OP2	-5.60	111.20	119.60
2	B	24	U	C2-N3-C4	-5.58	123.65	127.00
2	B	66	U	P-O3'-C3'	5.57	126.38	119.70
2	B	51	A	N1-C2-N3	-5.54	126.53	129.30
2	B	73	G	N7-C8-N9	-5.51	110.35	113.10
2	B	64	A	C8-N9-C4	5.44	107.97	105.80
2	B	44	C	C6-N1-C2	5.42	122.47	120.30
2	B	47	U	N3-C4-C5	5.42	117.85	114.60
2	B	72	C	C2-N3-C4	-5.41	117.19	119.90
2	B	48	G	C6-N1-C2	-5.40	121.86	125.10
2	B	46	C	N3-C4-N4	5.40	121.78	118.00
1	A	102	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	B	65	U	C5-C6-N1	-5.38	120.01	122.70
2	B	94	G	N1-C2-N3	-5.37	120.68	123.90
2	B	93	U	N1-C2-O2	-5.36	119.05	122.80
2	B	75	A	C5-C6-N1	-5.35	115.02	117.70
2	B	23	U	N3-C4-O4	5.34	123.14	119.40
3	C	9	DA	O4'-C1'-N9	5.33	111.73	108.00
2	B	14	C	N1-C2-O2	-5.30	115.72	118.90
2	B	50	A	N1-C2-N3	-5.29	126.66	129.30
1	A	650	ASP	CB-CG-OD1	5.28	123.06	118.30
2	B	49	U	N1-C2-O2	-5.28	119.10	122.80
2	B	13	G	OP2-P-O3'	5.24	116.74	105.20
1	A	58[A]	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	58[B]	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	5	A	OP1-P-OP2	-5.22	111.77	119.60
1	A	1404	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	B	68	U	N1-C2-O2	-5.20	119.16	122.80
3	C	9	DA	N1-C2-N3	-5.19	126.70	129.30
2	B	6	A	OP2-P-O3'	5.18	116.59	105.20
2	B	42	C	C6-N1-C2	5.17	122.37	120.30
2	B	21	G	N3-C2-N2	-5.16	116.29	119.90
2	B	44	C	N1-C1'-C2'	-5.15	106.34	112.00
2	B	20	G	C5-C6-N1	5.13	114.06	111.50
2	B	36	G	N9-C1'-C2'	-5.13	106.36	112.00
2	B	59	A	N1-C6-N6	5.11	121.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	U	OP2-P-O3'	5.09	116.41	105.20
2	B	14	C	N3-C2-O2	5.09	125.46	121.90
2	B	69	G	C6-N1-C2	-5.08	122.05	125.10
2	B	28	G	P-O3'-C3'	5.06	125.78	119.70
1	A	455	ARG	NE-CZ-NH1	-5.06	117.77	120.30
2	B	70	A	C6-N1-C2	5.06	121.63	118.60
2	B	16	C	N3-C4-C5	-5.04	119.89	121.90
2	B	62	G	N3-C4-C5	5.03	131.12	128.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	G	Sidechain

5.2 Too-close contacts ⓘ

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	11809	0	11590	101	0
2	B	1991	0	997	14	0
3	C	596	0	338	12	0
4	D	184	0	104	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	2	0	0	0	0
8	A	11	0	0	0	0
8	B	6	0	0	0	0
9	A	44	0	66	3	0
9	B	44	0	66	8	0
9	C	4	0	6	0	0
10	A	4	0	3	0	0
10	B	4	0	3	0	0
11	A	639	0	0	14	0
11	B	342	0	0	2	0
11	C	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	4	0	0	0	0
All	All	15757	0	13173	121	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 4.

All (121) 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:A:54[B]:ASN:OD1	1:A:58[B]:ARG:NH1	1.91	1.03
1:A:169:LYS:HB3	1:A:187:LEU:HD21	1.63	0.79
3:C:22:DT:H5"	3:C:22:DT:H6	1.46	0.79
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.64	0.78
1:A:578:LYS:NZ	1:A:582:GLU:OE2	2.17	0.77
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.06	0.74
1:A:1113:ASN:O	11:A:1802:HOH:O	2.09	0.70
1:A:723:LEU:HD12	1:A:727:LYS:HE3	1.72	0.70
1:A:1592:GLU:OE2	1:A:1595:LYS:NZ	2.23	0.70
3:C:22:DT:H5"	3:C:22:DT:C6	2.28	0.69
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.77	0.67
1:A:1594:LEU:HD12	1:A:1600:ILE:HD13	1.77	0.67
11:A:2317:HOH:O	9:B:116:EDO:H12	1.96	0.66
1:A:493:TYR:O	1:A:846:LYS:NZ	2.27	0.66
3:C:2:DC:H2'	3:C:3:DG:C8	2.30	0.66
1:A:693:LEU:HG	1:A:697:LYS:HE3	1.78	0.65
1:A:54[B]:ASN:HD21	1:A:58[B]:ARG:CZ	2.10	0.65
1:A:546:LYS:HE3	3:C:30:DC:H3'	1.79	0.65
1:A:645:GLY:HA2	9:A:1722:EDO:H11	1.79	0.65
1:A:1542:ILE:HD11	1:A:1575:TYR:HD2	1.62	0.64
1:A:58[A]:ARG:NH2	11:A:1806:HOH:O	2.30	0.63
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CE1	2.33	0.63
1:A:265:ASN:O	1:A:291:LEU:N	2.33	0.62
1:A:1592:GLU:HA	1:A:1595:LYS:HD3	1.82	0.61
1:A:1170:PHE:HD2	1:A:1212:ILE:HD13	1.66	0.60
3:C:4:DA:H2"	3:C:5:DT:H5"	1.84	0.60
3:C:24:DA:H8	3:C:24:DA:H5"	1.67	0.60
1:A:456:LYS:NZ	11:A:1809:HOH:O	2.34	0.60
1:A:1236:HIS:HE1	11:A:1996:HOH:O	1.85	0.59
1:A:1573:ILE:HD12	1:A:1594:LEU:HD23	1.86	0.58
1:A:1359:GLU:OE2	11:A:1803:HOH:O	2.17	0.57
1:A:1577:MET:HE1	1:A:1594:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:U:H4'	2:B:67:U:O5'	2.06	0.56
1:A:419:ASP:O	1:A:423[A]:GLU:HG3	2.06	0.55
1:A:23:PHE:HB2	9:A:1726:EDO:H22	1.89	0.54
2:B:94:G:C2	9:B:118:EDO:H11	2.43	0.54
1:A:129:ASP:OD1	1:A:129:ASP:N	2.38	0.54
1:A:173:LEU:O	1:A:177:ILE:HG22	2.07	0.54
1:A:659:HIS:HD2	11:B:236:HOH:O	1.89	0.54
1:A:109:ASP:OD1	1:A:109:ASP:N	2.42	0.53
1:A:1292[A]:CYS:SG	1:A:1360:PHE:HE2	2.32	0.52
3:C:21:DC:H2'	3:C:22:DT:C6	2.44	0.52
1:A:130:ILE:HG23	1:A:134:TYR:CE2	2.45	0.51
1:A:111:TYR:O	1:A:293:HIS:HE1	1.93	0.51
1:A:1233:PHE:CZ	2:B:66:U:H5'	2.45	0.51
1:A:620:ARG:HD3	11:A:2162:HOH:O	2.09	0.51
1:A:613:LYS:HG2	11:A:2268:HOH:O	2.10	0.50
1:A:982:ASN:CG	1:A:1131:ARG:HD3	2.31	0.50
1:A:1391:ILE:HG12	1:A:1396:LEU:HD11	1.94	0.50
1:A:45:LYS:HB3	1:A:911:VAL:HG12	1.94	0.50
9:B:119:EDO:H12	11:B:413:HOH:O	2.11	0.50
1:A:731:ALA:HB2	1:A:739:GLU:HB3	1.94	0.50
1:A:1436:LYS:NZ	11:A:1824:HOH:O	2.38	0.50
1:A:640:LYS:HE3	2:B:68:U:C6	2.47	0.50
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.45	0.49
1:A:12:LEU:HD11	1:A:1095[B]:PHE:CE2	2.48	0.49
1:A:983:ASP:HA	1:A:1129:ASN:HD22	1.78	0.49
1:A:351:LYS:NZ	11:A:1814:HOH:O	2.36	0.49
1:A:187:LEU:O	1:A:237:GLN:NE2	2.42	0.48
1:A:52:MET:SD	9:B:116:EDO:H22	2.52	0.48
1:A:1170:PHE:CD2	1:A:1212:ILE:HD13	2.48	0.48
2:B:94:G:C6	9:B:118:EDO:H11	2.49	0.48
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	1.96	0.48
1:A:10:ILE:HD13	1:A:1095[A]:PHE:HE2	1.79	0.48
1:A:130:ILE:HG22	1:A:137:GLU:OE2	2.13	0.48
1:A:1302:ILE:H	1:A:1302:ILE:HG12	1.55	0.48
1:A:514:VAL:O	1:A:529:ASP:HA	2.14	0.48
1:A:130:ILE:HG23	1:A:134:TYR:CD2	2.50	0.47
1:A:190:ILE:HG23	1:A:234:TYR:HB2	1.98	0.46
1:A:148:THR:HG22	1:A:301:ILE:HG21	1.98	0.46
2:B:66:U:H1'	2:B:67:U:OP2	2.15	0.45
1:A:664:LYS:NZ	11:A:1846:HOH:O	2.48	0.45
1:A:546:LYS:HE2	1:A:554:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:G:N1	9:B:118:EDO:H11	2.31	0.45
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.50	0.45
1:A:1583:LYS:NZ	3:C:4:DA:OP1	2.50	0.45
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CZ	2.52	0.44
1:A:1539:LEU:HB3	1:A:1544:ILE:HD12	1.99	0.44
1:A:4:LYS:HE2	1:A:23:PHE:CZ	2.53	0.44
1:A:266:PHE:HB2	1:A:295:VAL:CG2	2.48	0.44
1:A:1070:ASN:OD1	1:A:1072:ILE:HG12	2.17	0.44
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.33	0.44
1:A:622:ARG:HH22	3:C:30:DC:H4'	1.83	0.44
1:A:84:ASN:OD1	11:A:1804:HOH:O	2.21	0.44
1:A:856:ARG:HH21	1:A:856:ARG:HB3	1.82	0.44
1:A:1473:SER:HB3	4:D:2:DG:O4'	2.18	0.43
1:A:47:SER:HB3	1:A:1225:VAL:HA	2.00	0.43
3:C:4:DA:C2'	3:C:5:DT:H5''	2.47	0.43
1:A:866:ALA:HA	1:A:1095[B]:PHE:CE2	2.53	0.43
1:A:894:PRO:HB3	1:A:1122:PHE:HE1	1.82	0.43
1:A:983:ASP:HA	1:A:1129:ASN:ND2	2.33	0.43
1:A:12:LEU:HD21	1:A:1095[B]:PHE:CE1	2.53	0.43
1:A:264:PHE:CE2	1:A:292:HIS:HB2	2.54	0.43
2:B:25:U:H2'	2:B:26:C:C6	2.53	0.43
1:A:1231:GLU:HG3	11:A:1830:HOH:O	2.17	0.43
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.83	0.43
1:A:54[B]:ASN:ND2	11:A:1855:HOH:O	2.51	0.43
1:A:856:ARG:HB3	1:A:856:ARG:NH2	2.34	0.43
1:A:1171:CYS:SG	1:A:1212:ILE:HD12	2.59	0.42
3:C:11:DC:H2'	3:C:12:DC:C6	2.54	0.42
1:A:1595:LYS:HB2	1:A:1595:LYS:HE2	1.85	0.42
1:A:703:ILE:HD11	1:A:770:LEU:HD22	2.01	0.42
1:A:459:LYS:HG3	9:A:1722:EDO:O2	2.20	0.42
1:A:470:LEU:HB3	1:A:477:TRP:CD1	2.55	0.42
2:B:64:A:H1'	9:B:116:EDO:H21	2.02	0.42
1:A:493:TYR:CE1	1:A:544[A]:ARG:HG3	2.55	0.41
1:A:664:LYS:HA	1:A:667[B]:GLN:CG	2.50	0.41
1:A:1066:LEU:O	1:A:1073:LYS:HD2	2.19	0.41
1:A:890:GLN:HA	1:A:1116:LYS:HB3	2.02	0.41
1:A:663[B]:GLN:HG3	2:B:81:G:H5''	2.02	0.41
1:A:174:CYS:HB3	1:A:251:LEU:HB2	2.03	0.41
1:A:161:LEU:HD13	1:A:295:VAL:HB	2.03	0.41
1:A:1427:VAL:HG11	1:A:1438:ARG:HB2	2.03	0.41
4:D:3:DA:H2''	4:D:4:DT:H72	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:A:H2'	2:B:40:G:O4'	2.21	0.41
1:A:150:GLN:OE1	1:A:152:SER:N	2.54	0.40
1:A:452:ASN:HA	2:B:89:C:N3	2.36	0.40
1:A:1047:ARG:HD2	2:B:1:G:C6	2.56	0.40
2:B:89:C:H4'	9:B:117:EDO:H22	2.04	0.40
1:A:1091:THR:O	1:A:1095[B]:PHE:HD1	2.03	0.40
1:A:264:PHE:CD2	1:A:292:HIS:HB2	2.57	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	1445/1632 (88%)	1407 (97%)	37 (3%)	1 (0%)	56 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1128	GLY

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	1259/1484 (85%)	1226 (97%)	33 (3%)	54 32

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	109	ASP
1	A	127	LEU
1	A	129	ASP
1	A	133	ASP
1	A	162	MET
1	A	165	ILE
1	A	177	ILE
1	A	186	THR
1	A	259	LEU
1	A	310	ARG
1	A	351	LYS
1	A	551	LEU
1	A	626	LEU
1	A	723	LEU
1	A	730	ILE
1	A	791	ASN
1	A	846	LYS
1	A	856	ARG
1	A	987	LEU
1	A	1061	ARG
1	A	1068	ASP
1	A	1234	ASN
1	A	1301	SER
1	A	1302	ILE
1	A	1423	SER
1	A	1428	LYS
1	A	1511	ASN
1	A	1540	ARG
1	A	1563	LEU
1	A	1578	ASN
1	A	1580	SER
1	A	1614	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	293	HIS
1	A	342	ASN
1	A	488	GLN

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Mol	Chain	Res	Type
1	A	492	ASN
1	A	554	ASN
1	A	604	GLN
1	A	642	ASN
1	A	659	HIS
1	A	725	ASN
1	A	938	ASN
1	A	1051	ASN
1	A	1129	ASN
1	A	1157	GLN
1	A	1234	ASN
1	A	1236	HIS
1	A	1248	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 24 are monoatomic - leaving 25 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	$\# Z > 2$
9	EDO	A	1717	-	3,3,3	0.37	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	1718	-	3,3,3	0.47	0	2,2,2	0.82	0
9	EDO	A	1719	-	3,3,3	0.60	0	2,2,2	0.39	0
9	EDO	A	1720	-	3,3,3	1.00	0	2,2,2	0.21	0
9	EDO	A	1721	-	3,3,3	0.79	0	2,2,2	0.78	0
9	EDO	A	1722	-	3,3,3	0.41	0	2,2,2	0.80	0
9	EDO	A	1723	-	3,3,3	0.63	0	2,2,2	0.38	0
9	EDO	A	1724	-	3,3,3	0.58	0	2,2,2	0.16	0
9	EDO	A	1725	-	3,3,3	0.60	0	2,2,2	0.25	0
9	EDO	A	1726	-	3,3,3	0.47	0	2,2,2	0.34	0
9	EDO	A	1727	-	3,3,3	0.40	0	2,2,2	0.84	0
10	ACT	A	1728	-	0,3,3	0.00	-	0,3,3	0.00	-
9	EDO	B	109	-	3,3,3	0.56	0	2,2,2	0.51	0
9	EDO	B	110	-	3,3,3	0.68	0	2,2,2	0.85	0
9	EDO	B	111	-	3,3,3	0.66	0	2,2,2	0.23	0
9	EDO	B	112	-	3,3,3	0.80	0	2,2,2	0.14	0
9	EDO	B	113	-	3,3,3	0.48	0	2,2,2	0.33	0
9	EDO	B	114	-	3,3,3	0.72	0	2,2,2	0.35	0
9	EDO	B	115	-	3,3,3	0.59	0	2,2,2	0.16	0
9	EDO	B	116	-	3,3,3	0.40	0	2,2,2	0.77	0
9	EDO	B	117	-	3,3,3	0.55	0	2,2,2	0.37	0
9	EDO	B	118	-	3,3,3	0.36	0	2,2,2	0.42	0
9	EDO	B	119	-	3,3,3	0.49	0	2,2,2	0.27	0
10	ACT	B	120	-	0,3,3	0.00	-	0,3,3	0.00	-
9	EDO	C	101	-	3,3,3	0.57	0	2,2,2	0.24	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
9	EDO	A	1717	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1718	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1719	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1720	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1721	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1722	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1723	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1724	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1725	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1726	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1727	-	-	0/1/1/1	0/0/0/0
10	ACT	A	1728	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	109	-	-	0/1/1/1	0/0/0/0
9	EDO	B	110	-	-	0/1/1/1	0/0/0/0
9	EDO	B	111	-	-	0/1/1/1	0/0/0/0
9	EDO	B	112	-	-	0/1/1/1	0/0/0/0
9	EDO	B	113	-	-	0/1/1/1	0/0/0/0
9	EDO	B	114	-	-	0/1/1/1	0/0/0/0
9	EDO	B	115	-	-	0/1/1/1	0/0/0/0
9	EDO	B	116	-	-	0/1/1/1	0/0/0/0
9	EDO	B	117	-	-	0/1/1/1	0/0/0/0
9	EDO	B	118	-	-	0/1/1/1	0/0/0/0
9	EDO	B	119	-	-	0/1/1/1	0/0/0/0
10	ACT	B	120	-	-	0/0/0/0	0/0/0/0
9	EDO	C	101	-	-	0/1/1/1	0/0/0/0

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.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1722	EDO	2	0
9	A	1726	EDO	1	0
9	B	116	EDO	3	0
9	B	117	EDO	1	0
9	B	118	EDO	3	0
9	B	119	EDO	1	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 ⓘ

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	1455/1632 (89%)	0.83	262 (18%) 2 2	20, 44, 95, 129	0
2	B	94/94 (100%)	-0.21	0 100 100	20, 30, 59, 80	0
3	C	30/30 (100%)	0.01	2 (6%) 21 23	24, 46, 92, 133	0
4	D	9/9 (100%)	0.96	3 (33%) 0 0	39, 52, 111, 119	0
All	All	1588/1765 (89%)	0.75	267 (16%) 2 2	20, 43, 94, 133	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1542	ILE	10.9
1	A	1573	ILE	9.5
1	A	131	PHE	9.5
1	A	723	LEU	8.8
1	A	1565	TYR	8.8
1	A	1066	LEU	8.6
1	A	738	CYS	8.4
1	A	1564	ASP	8.3
1	A	127	LEU	8.0
1	A	256	THR	7.9
1	A	123	VAL	7.7
1	A	130	ILE	7.6
1	A	1566	VAL	7.6
1	A	177	ILE	7.5
1	A	1060	PHE	7.5
1	A	1072	ILE	7.4
1	A	1002	ILE	7.3
1	A	1567	ILE	6.9
1	A	168	PHE	6.9
1	A	1156	PRO	6.6
1	A	728	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	724	LEU	6.6
1	A	730	ILE	6.5
1	A	990	VAL	6.3
1	A	236	ILE	6.3
1	A	261	ILE	6.3
1	A	1065	PHE	6.3
1	A	940	ILE	6.3
1	A	187	LEU	6.2
1	A	429	THR	6.2
1	A	134	TYR	6.2
1	A	266	PHE	6.2
1	A	988	ILE	6.2
1	A	1053	THR	6.1
1	A	1005	LEU	6.1
1	A	1071	PRO	6.1
1	A	999	GLY	6.0
1	A	1598	THR	6.0
1	A	1064	LEU	6.0
1	A	175	THR	5.9
1	A	980	THR	5.9
1	A	1575	TYR	5.9
1	A	722	GLY	5.8
1	A	981	LEU	5.7
1	A	743	PHE	5.6
1	A	1563	LEU	5.5
1	A	841	ILE	5.5
1	A	111	TYR	5.4
1	A	264	PHE	5.4
1	A	1537	SER	5.4
1	A	1004	CYS	5.4
1	A	1059	ALA	5.4
1	A	729	ASN	5.3
1	A	843	LEU	5.3
1	A	126	ILE	5.3
1	A	742	ILE	5.3
1	A	1544	ILE	5.3
1	A	842	ILE	5.2
1	A	1003	PHE	5.1
1	A	125	ALA	5.1
1	A	1539	LEU	5.1
1	A	1077	ILE	5.1
1	A	1154	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	1049	PHE	5.0
1	A	967	LEU	5.0
1	A	1590	VAL	5.0
1	A	1592	GLU	4.9
1	A	972	PRO	4.9
1	A	188	LYS	4.9
1	A	203	ALA	4.8
1	A	1594	LEU	4.8
1	A	135	ASN	4.8
1	A	295	VAL	4.7
1	A	1050	ILE	4.7
1	A	720	ASN	4.6
1	A	1063	ALA	4.6
1	A	214	PHE	4.6
1	A	1052	LEU	4.5
1	A	1069	GLU	4.5
1	A	930	GLU	4.4
1	A	1046	TYR	4.4
1	A	186	THR	4.4
1	A	151	GLU	4.4
1	A	731	ALA	4.3
1	A	1621	GLY	4.3
1	A	1095[A]	PHE	4.3
1	A	1622	ILE	4.2
1	A	259	LEU	4.2
1	A	1067	ALA	4.2
1	A	1576	PHE	4.2
1	A	133	ASP	4.2
1	A	1593	ILE	4.2
1	A	165	ILE	4.1
1	A	200	ASP	4.1
1	A	1619	LEU	4.0
1	A	1155	LYS	3.9
1	A	759	TYR	3.9
1	A	124	LYS	3.9
1	A	1538	ASP	3.9
1	A	985	ALA	3.9
1	A	128	MET	3.8
1	A	1596	GLN	3.8
1	A	258	ASP	3.8
1	A	943	PHE	3.8
1	A	734	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1488	SER	3.8
1	A	294	PHE	3.8
1	A	211	THR	3.7
1	A	1187	ILE	3.7
1	A	1589	LYS	3.7
1	A	982	ASN	3.7
1	A	740	LYS	3.7
1	A	902	PHE	3.7
1	A	293	HIS	3.7
1	A	716	ILE	3.7
1	A	199	ALA	3.7
1	A	1076	VAL	3.7
1	A	739	GLU	3.6
1	A	1595	LYS	3.6
1	A	989	CYS	3.6
1	A	1574	ASN	3.6
1	A	726	HIS	3.5
1	A	1062	HIS	3.5
1	A	1153	GLY	3.5
1	A	973	ARG	3.5
1	A	298	VAL	3.5
1	A	1568	ASP	3.5
1	A	991	THR	3.5
1	A	1301	SER	3.5
1	A	733	ASN	3.5
1	A	257	ASP	3.5
4	D	9	DG	3.5
1	A	1191	TYR	3.5
1	A	1143	VAL	3.4
1	A	1073	LYS	3.4
1	A	639	HIS	3.4
1	A	195	PHE	3.4
1	A	1057	GLN	3.3
1	A	136	GLY	3.3
1	A	1543	GLY	3.3
1	A	516	TYR	3.3
1	A	190	ILE	3.3
1	A	1074	GLN	3.3
1	A	296	PHE	3.3
1	A	291	LEU	3.3
1	A	235	ASN	3.3
1	A	166	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1070	ASN	3.2
1	A	1487	ILE	3.2
1	A	30	LEU	3.2
1	A	143	TYR	3.2
1	A	969	HIS	3.1
1	A	1194	TYR	3.1
1	A	160	LYS	3.1
1	A	254	LEU	3.1
1	A	1540	ARG	3.1
1	A	855	THR	3.0
1	A	783	PHE	3.0
1	A	746	ILE	3.0
1	A	932	ILE	3.0
1	A	173	LEU	3.0
1	A	747	CYS	3.0
1	A	1139	LEU	3.0
1	A	1006	ARG	3.0
1	A	174	CYS	3.0
4	D	8	DG	3.0
1	A	112	SER	3.0
1	A	1068	ASP	2.9
1	A	171	MET	2.9
1	A	1614	MET	2.9
1	A	1061	ARG	2.9
1	A	928	SER	2.9
1	A	176	ASP	2.9
1	A	933	PHE	2.9
1	A	191	THR	2.9
1	A	297	ALA	2.9
1	A	986	ASN	2.9
1	A	971	ILE	2.9
1	A	719	ASP	2.8
1	A	936	LYS	2.8
1	A	255	LEU	2.8
1	A	179	ASP	2.8
1	A	260	ASP	2.8
1	A	155	SER	2.8
1	A	736	GLY	2.8
1	A	1616	GLY	2.8
1	A	732	ARG	2.8
1	A	109	ASP	2.8
1	A	1078	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	253	THR	2.7
1	A	237	GLN	2.7
1	A	1536	PRO	2.7
1	A	234	TYR	2.6
1	A	1055	GLN	2.6
1	A	1577	MET	2.6
1	A	156	GLU	2.6
1	A	1534	GLU	2.6
1	A	152	SER	2.6
1	A	241	LYS	2.6
1	A	776	ASN	2.6
1	A	935	ASP	2.6
1	A	966	GLU	2.6
1	A	1000	ASN	2.6
1	A	814	CYS	2.6
1	A	129	ASP	2.6
1	A	142	SER	2.6
1	A	265	ASN	2.6
1	A	201	TYR	2.6
1	A	939	ARG	2.5
1	A	189	GLU	2.5
1	A	2	ASN	2.5
1	A	987	LEU	2.5
1	A	132	ASP	2.5
1	A	65	ILE	2.5
1	A	146	LEU	2.5
1	A	931	ASN	2.5
1	A	1578	ASN	2.5
1	A	854	PRO	2.4
1	A	1054	PRO	2.4
1	A	263	ASN	2.4
1	A	929	PRO	2.4
1	A	1620	ALA	2.4
1	A	785	ARG	2.4
4	D	7	DC	2.4
1	A	1082	ASN	2.4
1	A	178	LYS	2.4
1	A	1523	PHE	2.4
1	A	924	LEU	2.3
1	A	778	ALA	2.3
1	A	292	HIS	2.3
1	A	856	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	735	LYS	2.3
1	A	781	PRO	2.3
1	A	238	GLU	2.3
1	A	262	TRP	2.3
1	A	1571	SER	2.3
1	A	1192	SER	2.2
1	A	970	ILE	2.2
1	A	1597	SER	2.2
1	A	33	LEU	2.2
1	A	31	GLU	2.2
1	A	919	ARG	2.1
1	A	1151	ALA	2.1
3	C	1	DC	2.1
1	A	212	GLN	2.1
1	A	428	VAL	2.1
1	A	853	ILE	2.1
1	A	1541	ASP	2.1
1	A	1056	GLU	2.1
1	A	921	LYS	2.1
1	A	1209	PHE	2.1
1	A	150	GLN	2.1
1	A	737	LYS	2.1
1	A	53[A]	ASN	2.1
3	C	2	DC	2.1
1	A	1094	TYR	2.1
1	A	1157	GLN	2.1
1	A	1	MET	2.1
1	A	322	VAL	2.1
1	A	794	TYR	2.0
1	A	1243	GLY	2.0
1	A	213	LYS	2.0
1	A	937	ASN	2.0
1	A	147	ALA	2.0
1	A	1560	ARG	2.0
1	A	1486	ASP	2.0
1	A	110	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	ACT	B	120	4/4	0.94	0.18	5.33	76,77,77,77	0
9	EDO	B	115	4/4	0.92	0.10	3.13	43,47,52,55	0
9	EDO	B	114	4/4	0.85	0.19	2.98	46,49,52,52	0
9	EDO	A	1726	4/4	0.94	0.14	2.80	49,49,56,58	0
9	EDO	B	110	4/4	0.95	0.11	2.56	32,33,33,37	0
9	EDO	A	1724	4/4	0.91	0.12	2.26	44,45,45,46	0
9	EDO	A	1727	4/4	0.78	0.18	1.68	62,62,63,65	0
9	EDO	A	1721	4/4	0.90	0.15	1.00	32,32,36,36	0
9	EDO	A	1718	4/4	0.95	0.12	0.75	36,40,43,48	0
9	EDO	B	112	4/4	0.98	0.11	0.57	28,29,32,32	0
9	EDO	B	109	4/4	0.97	0.09	0.55	30,31,33,36	0
9	EDO	A	1722	4/4	0.92	0.17	0.42	48,49,52,53	0
9	EDO	B	117	4/4	0.89	0.13	0.32	43,45,46,46	0
5	ZN	A	1701	1/1	0.99	0.13	0.17	26,26,26,26	0
10	ACT	A	1728	4/4	0.96	0.11	0.11	32,33,34,35	0
9	EDO	A	1719	4/4	0.96	0.07	-0.06	31,34,37,39	0
9	EDO	A	1720	4/4	0.92	0.15	-0.15	30,36,38,39	0
8	CA	A	1715	1/1	0.98	0.08	-0.24	52,52,52,52	0
9	EDO	A	1723	4/4	0.97	0.08	-0.24	27,32,37,42	0
7	CL	A	1705	1/1	0.99	0.09	-0.24	28,28,28,28	0
9	EDO	C	101	4/4	0.88	0.13	-0.38	45,49,50,52	0
9	EDO	B	111	4/4	0.98	0.13	-0.40	23,24,24,27	0
9	EDO	B	116	4/4	0.92	0.13	-0.49	37,47,50,51	0
8	CA	B	108	1/1	0.93	0.11	-0.55	80,80,80,80	0
9	EDO	B	113	4/4	0.93	0.08	-0.55	36,36,39,40	0
7	CL	A	1704	1/1	0.98	0.06	-0.79	43,43,43,43	0
8	CA	A	1706	1/1	0.97	0.05	-1.12	67,67,67,67	0
6	NA	A	1702	1/1	0.95	0.07	-1.19	43,43,43,43	0
8	CA	B	103	1/1	0.99	0.05	-1.49	33,33,33,33	0
6	NA	B	101	1/1	1.00	0.07	-1.76	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	EDO	A	1717	4/4	0.97	0.08	-1.77	40,42,44,45	0
8	CA	A	1709	1/1	0.99	0.07	-3.63	50,50,50,50	0
9	EDO	A	1725	4/4	0.70	0.17	-	60,61,61,62	0
8	CA	A	1708	1/1	0.98	0.04	-	42,42,42,42	0
8	CA	B	106	1/1	0.93	0.07	-	54,54,54,54	0
9	EDO	B	119	4/4	0.85	0.20	-	44,46,47,49	0
8	CA	B	107	1/1	0.92	0.09	-	84,84,84,84	0
8	CA	A	1713	1/1	0.90	0.12	-	96,96,96,96	0
8	CA	B	104	1/1	0.88	0.05	-	73,73,73,73	0
8	CA	A	1707	1/1	1.00	0.03	-	34,34,34,34	0
8	CA	A	1710	1/1	0.94	0.09	-	48,48,48,48	0
8	CA	A	1712	1/1	0.95	0.11	-	61,61,61,61	0
6	NA	A	1703	1/1	0.87	0.08	-	61,61,61,61	0
9	EDO	B	118	4/4	0.84	0.18	-	56,57,58,58	0
8	CA	B	105	1/1	0.99	0.06	-	35,35,35,35	0
6	NA	B	102	1/1	0.95	0.15	-	46,46,46,46	0
8	CA	A	1711	1/1	0.92	0.06	-	79,79,79,79	0
8	CA	A	1714	1/1	0.96	0.13	-	60,60,60,60	0
8	CA	A	1716	1/1	0.96	0.08	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.