



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:06 am BST

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](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.

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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 : 2.11  
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) : 2.11

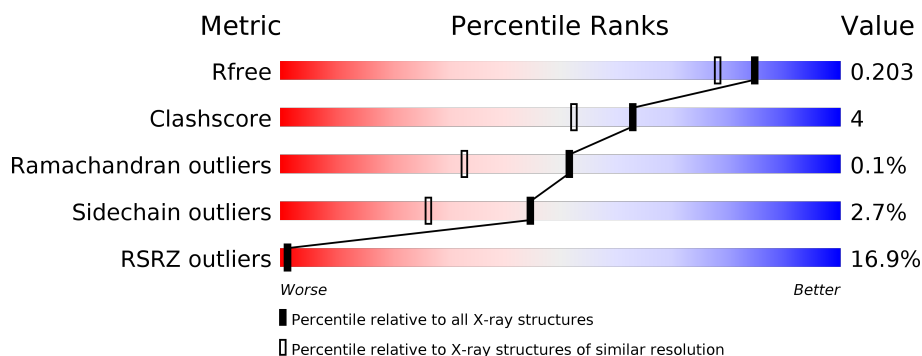
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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  $\geq 3$ , 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	1632	
2	B	94	
3	C	30	
4	D	9	

## 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

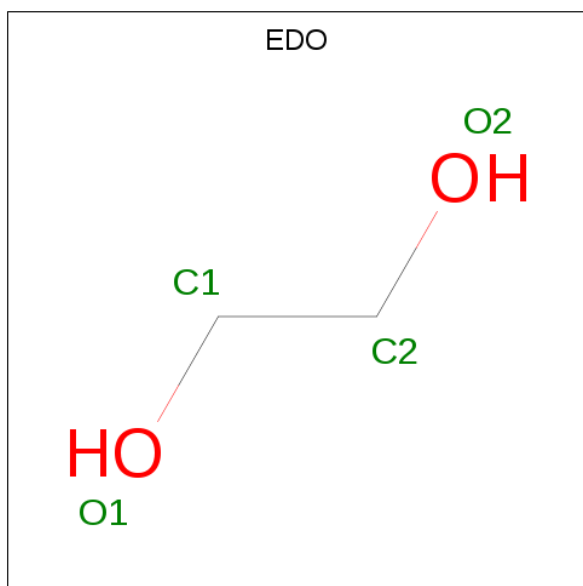
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



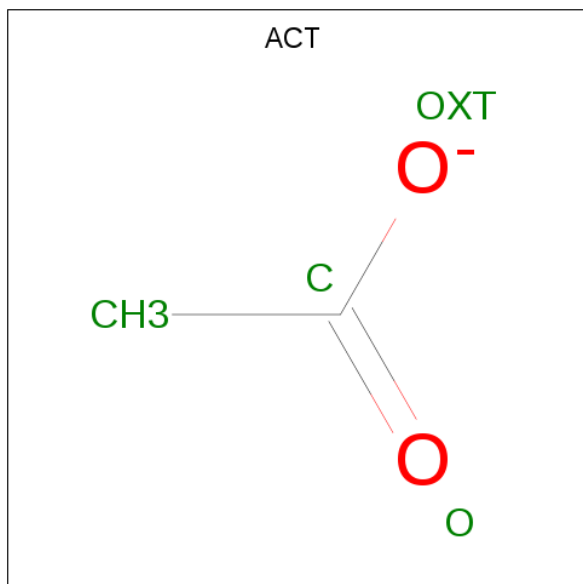
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0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

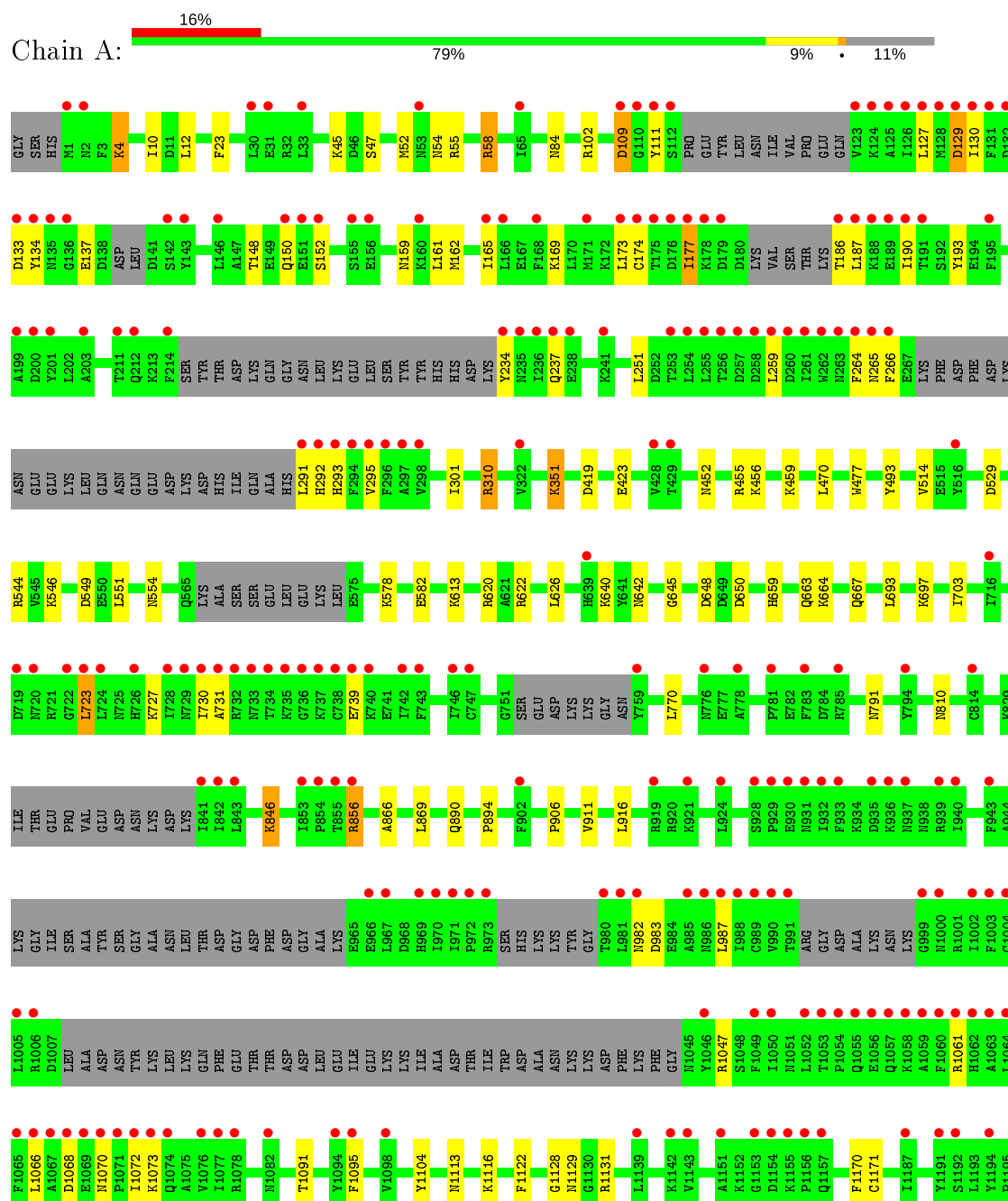
- Molecule 11 is water.

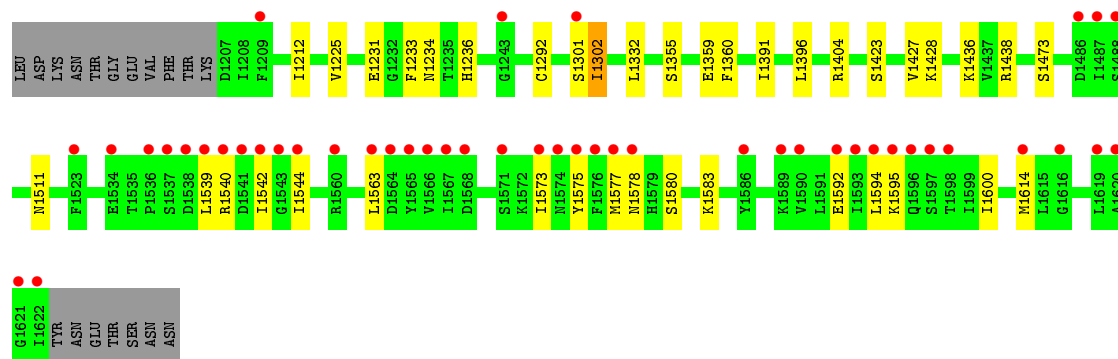
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	639	Total	O	0	0
			639	639		
11	B	342	Total	O	0	0
			342	342		
11	C	68	Total	O	0	0
			68	68		
11	D	4	Total	O	0	0
			4	4		

### 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 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.

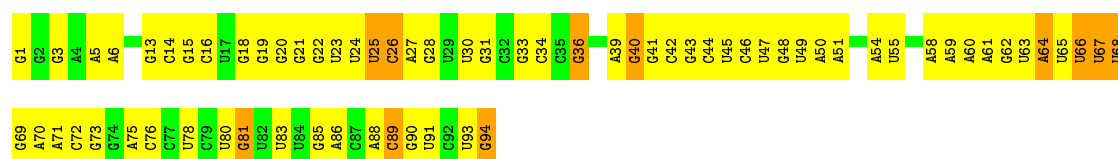
- Molecule 1: CRISPR-associated endonuclease Cas9





- Molecule 2: Guide RNA

Chain B: 27% 62% 12%



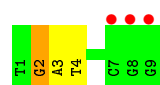
- Molecule 3: Target DNA

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10 _2155: ???	Depositor
R, $R_{free}$	0.180 , 0.203 0.180 , 0.203	Depositor DCC
$R_{free}$ test set	12766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 ⓘ

### 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:546:LYS:HE3	3:C:30:DC:H3'	1.79	0.65
1:A:54[B]:ASN:HD21	1:A:58[B]:ARG:CZ	2.10	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:HH22	3:C:30:DC:H4'	1.83	0.44
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.33	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:47:SER:HB3	1:A:1225:VAL:HA	2.00	0.43
1:A:1473:SER:HB3	4:D:2:DG:O4'	2.18	0.43
3:C:4:DA:C2'	3:C:5:DT:H5''	2.47	0.43
1:A:894:PRO:HB3	1:A:1122:PHE:HE1	1.82	0.43
1:A:866:ALA:HA	1:A:1095[B]:PHE:CE2	2.53	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:1047:ARG:HD2	2:B:1:G:C6	2.56	0.40
1:A:452:ASN:HA	2:B:89:C:N3	2.36	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%)	51 33

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%)	46 28

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	1726	-	3,3,3	0.48	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	B	110	-	3,3,3	0.72	0	2,2,2	0.77	0
9	EDO	B	111	-	3,3,3	0.69	0	2,2,2	0.24	0
9	EDO	A	1720	-	3,3,3	1.05	0	2,2,2	0.15	0
9	EDO	A	1718	-	3,3,3	0.48	0	2,2,2	0.74	0
9	EDO	A	1717	-	3,3,3	0.38	0	2,2,2	0.76	0
9	EDO	A	1719	-	3,3,3	0.62	0	2,2,2	0.40	0
10	ACT	B	120	-	1,3,3	1.67	0	0,3,3	0.00	-
9	EDO	B	109	-	3,3,3	0.57	0	2,2,2	0.44	0
9	EDO	B	119	-	3,3,3	0.51	0	2,2,2	0.29	0
9	EDO	B	113	-	3,3,3	0.50	0	2,2,2	0.29	0
9	EDO	A	1722	-	3,3,3	0.43	0	2,2,2	0.71	0
9	EDO	A	1723	-	3,3,3	0.65	0	2,2,2	0.33	0
9	EDO	B	115	-	3,3,3	0.61	0	2,2,2	0.17	0
9	EDO	B	118	-	3,3,3	0.36	0	2,2,2	0.39	0
9	EDO	C	101	-	3,3,3	0.59	0	2,2,2	0.27	0
10	ACT	A	1728	-	1,3,3	1.13	0	0,3,3	0.00	-
9	EDO	A	1725	-	3,3,3	0.62	0	2,2,2	0.26	0
9	EDO	A	1721	-	3,3,3	0.84	0	2,2,2	0.71	0
9	EDO	B	114	-	3,3,3	0.75	0	2,2,2	0.38	0
9	EDO	A	1727	-	3,3,3	0.41	0	2,2,2	0.75	0
9	EDO	A	1724	-	3,3,3	0.61	0	2,2,2	0.18	0
9	EDO	B	116	-	3,3,3	0.41	0	2,2,2	0.69	0
9	EDO	B	117	-	3,3,3	0.56	0	2,2,2	0.32	0
9	EDO	B	112	-	3,3,3	0.83	0	2,2,2	0.11	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	1726	-	-	0/1/1/1	-
9	EDO	B	110	-	-	1/1/1/1	-
9	EDO	B	111	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1717	-	-	1/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	B	109	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	A	1722	-	-	1/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	115	-	-	1/1/1/1	-
9	EDO	B	118	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	A	1721	-	-	0/1/1/1	-
9	EDO	B	114	-	-	0/1/1/1	-
9	EDO	C	101	-	-	0/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	B	116	-	-	0/1/1/1	-
9	EDO	B	117	-	-	1/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1725	EDO	O1-C1-C2-O2
9	B	110	EDO	O1-C1-C2-O2
9	B	115	EDO	O1-C1-C2-O2
9	B	117	EDO	O1-C1-C2-O2
9	A	1717	EDO	O1-C1-C2-O2
9	A	1722	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 11 short contacts:

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

## 5.7 Other polymers ⓘ

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, 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	1455/1632 (89%)	0.83	264 (18%) ⓘ ⓘ	20, 44, 95, 129	0
2	B	94/94 (100%)	-0.21	0 ⓘ ⓘ	20, 30, 59, 80	0
3	C	30/30 (100%)	0.01	2 (6%) ⓘ ⓘ	24, 46, 92, 133	0
4	D	9/9 (100%)	0.96	3 (33%) ⓘ ⓘ	39, 52, 111, 119	0
All	All	1588/1765 (89%)	0.75	269 (16%) ⓘ ⓘ	20, 43, 94, 133	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1542	ILE	10.9
1	A	1573	ILE	9.6
1	A	131	PHE	9.4
1	A	1066	LEU	9.0
1	A	723	LEU	8.7
1	A	1565	TYR	8.7
1	A	738	CYS	8.4
1	A	1564	ASP	8.2
1	A	127	LEU	8.0
1	A	256	THR	7.9
1	A	123	VAL	7.9
1	A	1566	VAL	7.6
1	A	177	ILE	7.6
1	A	130	ILE	7.6
1	A	1060	PHE	7.5
1	A	1072	ILE	7.5
1	A	1002	ILE	7.2
1	A	168	PHE	6.9
1	A	1567	ILE	6.8
1	A	724	LEU	6.7
1	A	728	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	1156	PRO	6.6
1	A	730	ILE	6.5
1	A	236	ILE	6.4
1	A	1065	PHE	6.4
1	A	990	VAL	6.4
1	A	261	ILE	6.3
1	A	266	PHE	6.3
1	A	988	ILE	6.3
1	A	429	THR	6.3
1	A	187	LEU	6.2
1	A	134	TYR	6.2
1	A	940	ILE	6.2
1	A	1053	THR	6.1
1	A	1005	LEU	6.1
1	A	1071	PRO	6.0
1	A	999	GLY	6.0
1	A	1598	THR	6.0
1	A	175	THR	6.0
1	A	1064	LEU	5.9
1	A	1575	TYR	5.9
1	A	980	THR	5.9
1	A	722	GLY	5.8
1	A	981	LEU	5.8
1	A	743	PHE	5.7
1	A	1563	LEU	5.5
1	A	111	TYR	5.5
1	A	264	PHE	5.5
1	A	1059	ALA	5.4
1	A	841	ILE	5.4
1	A	843	LEU	5.4
1	A	729	ASN	5.3
1	A	1004	CYS	5.3
1	A	1537	SER	5.3
1	A	742	ILE	5.3
1	A	126	ILE	5.3
1	A	842	ILE	5.3
1	A	1544	ILE	5.3
1	A	1003	PHE	5.2
1	A	125	ALA	5.1
1	A	1539	LEU	5.1
1	A	1049	PHE	5.1
1	A	1077	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	1154	ASP	5.0
1	A	1590	VAL	5.0
1	A	967	LEU	5.0
1	A	972	PRO	5.0
1	A	188	LYS	4.9
1	A	1592	GLU	4.9
1	A	1594	LEU	4.9
1	A	203	ALA	4.8
1	A	135	ASN	4.8
1	A	1050	ILE	4.7
1	A	295	VAL	4.6
1	A	720	ASN	4.6
1	A	1069	GLU	4.5
1	A	1052	LEU	4.5
1	A	214	PHE	4.5
1	A	1063	ALA	4.5
1	A	1046	TYR	4.5
1	A	186	THR	4.4
1	A	930	GLU	4.4
1	A	1576	PHE	4.4
1	A	151	GLU	4.4
1	A	731	ALA	4.3
1	A	1621	GLY	4.3
1	A	1622	ILE	4.3
1	A	1095[A]	PHE	4.2
1	A	259	LEU	4.2
1	A	165	ILE	4.2
1	A	1067	ALA	4.2
1	A	133	ASP	4.2
1	A	1593	ILE	4.1
1	A	200	ASP	4.1
1	A	1619	LEU	4.0
1	A	124	LYS	3.9
1	A	1155	LYS	3.9
1	A	985	ALA	3.9
1	A	759	TYR	3.9
1	A	1596	GLN	3.8
1	A	258	ASP	3.8
1	A	1538	ASP	3.8
1	A	943	PHE	3.8
1	A	1187	ILE	3.8
1	A	734	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	982	ASN	3.8
1	A	294	PHE	3.8
1	A	128	MET	3.8
1	A	1488	SER	3.7
1	A	740	LYS	3.7
1	A	211	THR	3.7
1	A	1589	LYS	3.7
1	A	989	CYS	3.7
1	A	199	ALA	3.7
1	A	716	ILE	3.7
1	A	293	HIS	3.7
1	A	739	GLU	3.6
1	A	902	PHE	3.6
1	A	1595	LYS	3.6
1	A	1076	VAL	3.6
1	A	298	VAL	3.6
1	A	1153	GLY	3.6
1	A	726	HIS	3.5
1	A	1574	ASN	3.5
1	A	1301	SER	3.5
1	A	973	ARG	3.5
1	A	991	THR	3.5
1	A	1191	TYR	3.5
1	A	1062	HIS	3.5
1	A	733	ASN	3.5
1	A	257	ASP	3.5
4	D	9	DG	3.5
1	A	1073	LYS	3.4
1	A	1143	VAL	3.4
1	A	1568	ASP	3.4
1	A	1057	GLN	3.4
1	A	639	HIS	3.4
1	A	195	PHE	3.4
1	A	136	GLY	3.3
1	A	190	ILE	3.3
1	A	1543	GLY	3.3
1	A	296	PHE	3.2
1	A	166	LEU	3.2
1	A	1074	GLN	3.2
1	A	143	TYR	3.2
1	A	516	TYR	3.2
1	A	291	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1070	ASN	3.2
1	A	235	ASN	3.2
1	A	1487	ILE	3.2
1	A	30	LEU	3.2
1	A	254	LEU	3.2
1	A	160	LYS	3.1
1	A	173	LEU	3.1
1	A	1194	TYR	3.1
1	A	1540	ARG	3.1
1	A	747	CYS	3.0
1	A	855	THR	3.0
1	A	969	HIS	3.0
1	A	1139	LEU	3.0
1	A	746	ILE	3.0
1	A	783	PHE	3.0
1	A	932	ILE	3.0
1	A	1006	ARG	3.0
1	A	112	SER	3.0
4	D	8	DG	3.0
1	A	297	ALA	3.0
1	A	971	ILE	3.0
1	A	1614	MET	3.0
1	A	174	CYS	3.0
1	A	1068	ASP	3.0
1	A	171	MET	2.9
1	A	1061	ARG	2.9
1	A	255	LEU	2.9
1	A	936	LYS	2.9
1	A	933	PHE	2.8
1	A	176	ASP	2.8
1	A	736	GLY	2.8
1	A	986	ASN	2.8
1	A	191	THR	2.8
1	A	719	ASP	2.8
1	A	155	SER	2.8
1	A	260	ASP	2.8
1	A	928	SER	2.8
1	A	732	ARG	2.8
1	A	109	ASP	2.8
1	A	1078	ARG	2.7
1	A	253	THR	2.7
1	A	179	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1616	GLY	2.7
1	A	1577	MET	2.7
1	A	237	GLN	2.7
1	A	156	GLU	2.6
1	A	241	LYS	2.6
1	A	1534	GLU	2.6
1	A	234	TYR	2.6
1	A	152	SER	2.6
1	A	935	ASP	2.6
1	A	265	ASN	2.6
1	A	1536	PRO	2.6
1	A	189	GLU	2.6
1	A	1055	GLN	2.6
1	A	129	ASP	2.6
1	A	776	ASN	2.6
1	A	966	GLU	2.6
1	A	2	ASN	2.6
1	A	201	TYR	2.6
1	A	814	CYS	2.6
1	A	939	ARG	2.5
1	A	132	ASP	2.5
1	A	142	SER	2.5
1	A	146	LEU	2.5
1	A	987	LEU	2.5
1	A	1000	ASN	2.5
1	A	65	ILE	2.5
1	A	1578	ASN	2.5
1	A	931	ASN	2.5
1	A	854	PRO	2.4
1	A	929	PRO	2.4
1	A	1620	ALA	2.4
1	A	1082	ASN	2.4
1	A	1054	PRO	2.4
1	A	178	LYS	2.4
1	A	778	ALA	2.4
1	A	785	ARG	2.4
1	A	263	ASN	2.4
4	D	7	DC	2.4
1	A	1523	PHE	2.4
1	A	292	HIS	2.4
1	A	856	ARG	2.3
1	A	781	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	2.3
1	A	735	LYS	2.3
1	A	238	GLU	2.3
1	A	1192	SER	2.3
1	A	1571	SER	2.2
1	A	924	LEU	2.2
1	A	33	LEU	2.2
1	A	1597	SER	2.2
1	A	970	ILE	2.2
1	A	31	GLU	2.2
1	A	1151	ALA	2.2
1	A	919	ARG	2.1
3	C	1	DC	2.1
1	A	737	LYS	2.1
1	A	1209	PHE	2.1
1	A	921	LYS	2.1
1	A	1094	TYR	2.1
1	A	428	VAL	2.1
1	A	1541	ASP	2.1
1	A	212	GLN	2.1
1	A	1157	GLN	2.1
1	A	853	ILE	2.1
3	C	2	DC	2.1
1	A	1056	GLU	2.1
1	A	794	TYR	2.1
1	A	322	VAL	2.1
1	A	53[A]	ASN	2.1
1	A	937	ASN	2.1
1	A	1560	ARG	2.0
1	A	1	MET	2.0
1	A	1243	GLY	2.0
1	A	150	GLN	2.0
1	A	110	GLY	2.0
1	A	1058	LYS	2.0
1	A	1142	LYS	2.0
1	A	1586	TYR	2.0
1	A	1098	VAL	2.0
1	A	1486	ASP	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. 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( $\text{\AA}^2$ )	Q<0.9
9	EDO	A	1725	4/4	0.70	0.17	60,61,61,62	0
9	EDO	A	1727	4/4	0.78	0.18	62,62,63,65	0
9	EDO	B	118	4/4	0.84	0.18	56,57,58,58	0
9	EDO	B	119	4/4	0.85	0.20	44,46,47,49	0
9	EDO	B	114	4/4	0.85	0.19	46,49,52,52	0
9	EDO	C	101	4/4	0.87	0.14	45,49,50,52	0
6	NA	A	1703	1/1	0.87	0.08	61,61,61,61	0
8	CA	B	104	1/1	0.88	0.05	73,73,73,73	0
9	EDO	A	1721	4/4	0.90	0.15	32,32,36,36	0
8	CA	A	1713	1/1	0.90	0.12	96,96,96,96	0
9	EDO	B	117	4/4	0.90	0.13	43,45,46,46	0
9	EDO	A	1724	4/4	0.91	0.11	44,45,45,46	0
9	EDO	A	1722	4/4	0.92	0.17	48,49,52,53	0
9	EDO	A	1720	4/4	0.92	0.15	30,36,38,39	0
9	EDO	B	116	4/4	0.92	0.13	37,47,50,51	0
8	CA	B	107	1/1	0.92	0.09	84,84,84,84	0
8	CA	A	1711	1/1	0.92	0.06	79,79,79,79	0
8	CA	B	108	1/1	0.93	0.11	80,80,80,80	0
9	EDO	B	115	4/4	0.93	0.10	43,47,52,55	0
9	EDO	B	113	4/4	0.93	0.09	36,36,39,40	0
10	ACT	B	120	4/4	0.94	0.18	76,77,77,77	0
9	EDO	A	1726	4/4	0.94	0.14	49,49,56,58	0
8	CA	B	106	1/1	0.94	0.07	54,54,54,54	0
8	CA	A	1710	1/1	0.94	0.09	48,48,48,48	0
6	NA	A	1702	1/1	0.95	0.08	43,43,43,43	0
8	CA	A	1712	1/1	0.95	0.11	61,61,61,61	0
9	EDO	B	110	4/4	0.95	0.11	32,33,33,37	0
6	NA	B	102	1/1	0.95	0.15	46,46,46,46	0
9	EDO	A	1718	4/4	0.95	0.12	36,40,43,48	0
9	EDO	A	1719	4/4	0.96	0.07	31,34,37,39	0
8	CA	A	1714	1/1	0.96	0.13	60,60,60,60	0
10	ACT	A	1728	4/4	0.96	0.11	32,33,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CA	A	1716	1/1	0.96	0.08	56,56,56,56	0
9	EDO	A	1717	4/4	0.97	0.08	40,42,44,45	0
9	EDO	A	1723	4/4	0.97	0.08	27,32,37,42	0
9	EDO	B	109	4/4	0.97	0.09	30,31,33,36	0
8	CA	A	1706	1/1	0.97	0.05	67,67,67,67	0
7	CL	A	1704	1/1	0.98	0.06	43,43,43,43	0
8	CA	A	1715	1/1	0.98	0.08	52,52,52,52	0
9	EDO	B	112	4/4	0.98	0.11	28,29,32,32	0
9	EDO	B	111	4/4	0.98	0.13	23,24,24,27	0
8	CA	A	1708	1/1	0.98	0.04	42,42,42,42	0
7	CL	A	1705	1/1	0.99	0.09	28,28,28,28	0
8	CA	B	105	1/1	0.99	0.06	35,35,35,35	0
8	CA	A	1709	1/1	0.99	0.07	50,50,50,50	0
5	ZN	A	1701	1/1	0.99	0.13	26,26,26,26	0
8	CA	B	103	1/1	0.99	0.05	33,33,33,33	0
8	CA	A	1707	1/1	1.00	0.03	34,34,34,34	0
6	NA	B	101	1/1	1.00	0.07	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.