



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 10, 2019 – 11:58 PM EST

PDB ID : 6NQB  
EMDB ID: : EMD-0482  
Title : Role of Era in Assembly and Homeostasis of the Ribosomal Small Subunit  
Authors : Ortega, J.  
Deposited on : 2019-01-20  
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

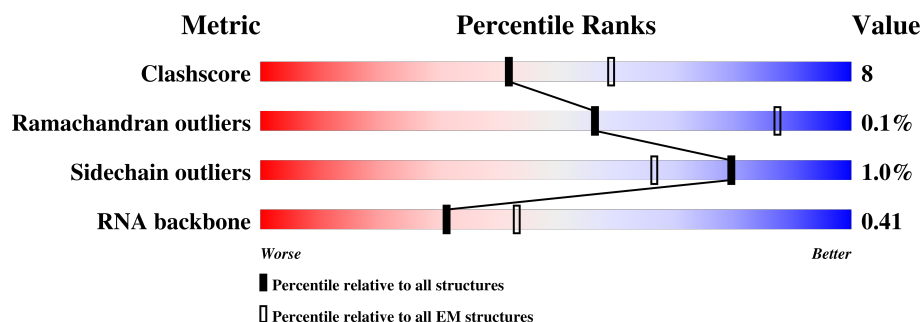
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	C	206	77% 23%
2	J	98	74% 24% .
3	N	99	76% 19% . .
4	S	74	70% 30%
5	A	1542	38% 38% 10% 13%
6	D	205	79% 20% .
7	E	149	82% 18%
8	F	93	71% 12% 17%

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Mol	Chain	Length	Quality of chain
9	H	129	 79%21%
10	L	123	 84%15%.
11	O	86	 83%15%.
12	P	79	 81%15%.
13	Q	79	 85%15%
14	R	52	 67%27%6%
15	T	85	 78%22%
16	B	217	 83%17%

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 42570 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 2 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 3 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLU	deletion	UNP A0A090BZT4

- Molecule 4 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	74	Total	C	N	O	S	0	0
			594	381	110	101	2		

- Molecule 5 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1341	Total	C	N	O	P	0	0
			28767	12830	5276	9320	1341		

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	149	Total	C	N	O	S	0	0
			1089	675	209	199	6		

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	77	Total	C	N	O	S	0	0
			630	401	109	114	6		

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 11 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	86	Total	C	N	O	S	0	0
			698	431	141	125	1		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 13 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	R	49	Total	C	N	O	0	0
			405	258	76	71		

- Molecule 15 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	85	Total	C	N	O	S	0	0
			659	408	134	114	3		

- Molecule 16 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	217	Total	C	N	O	S	0	0
			1696	1076	304	310	6		

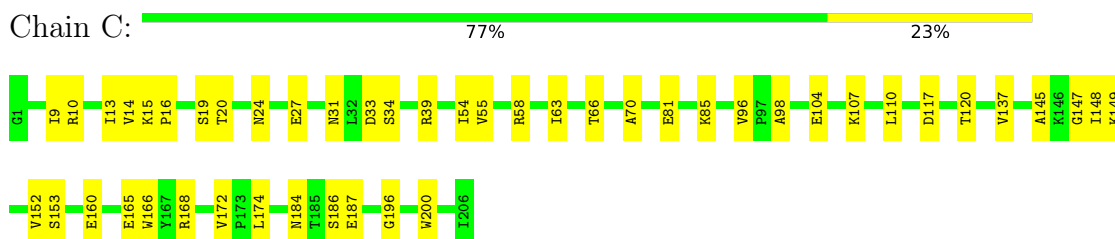
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	

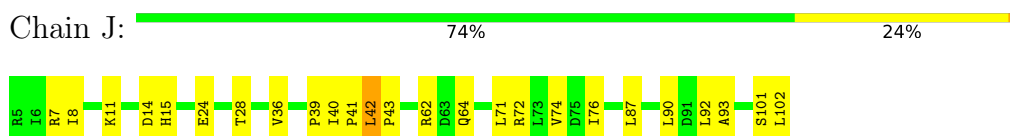
### 3 Residue-property plots

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. 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. 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.

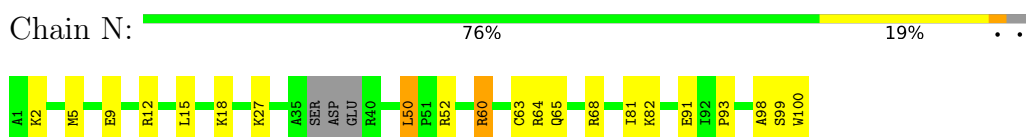
- Molecule 1: 30S ribosomal protein S3



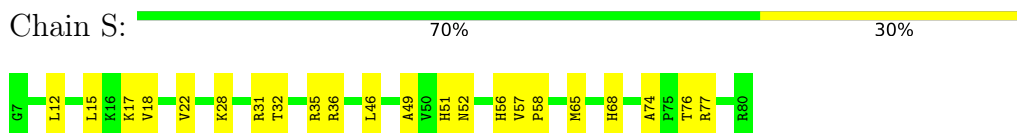
- Molecule 2: 30S ribosomal protein S10



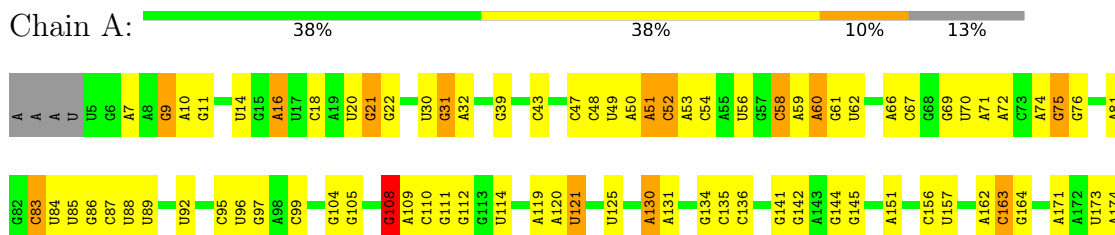
- Molecule 3: 30S ribosomal protein S14



- Molecule 4: 30S ribosomal protein S19



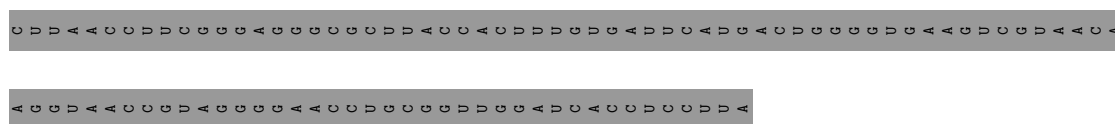
- Molecule 5: 16S RIBOSOMAL RNA



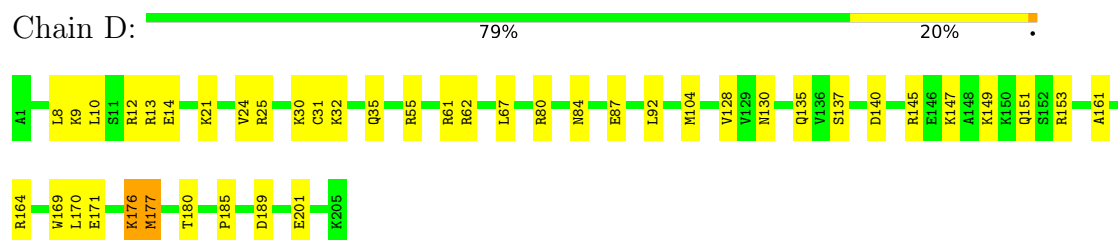

**WORLDWIDE PDB**  
 PROTEIN DATA BANK  

**EMDataBank**  
 Unified Data Resource for 3DEM

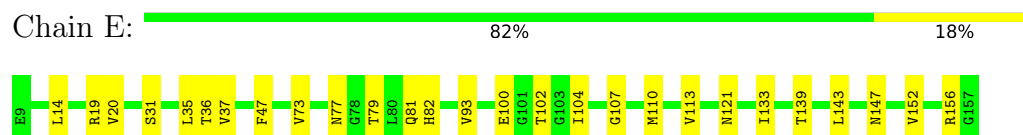




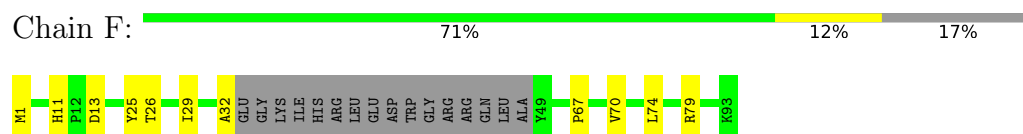
• Molecule 6: 30S ribosomal protein S4



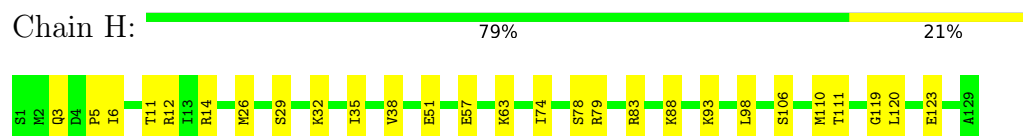
• Molecule 7: 30S ribosomal protein S5



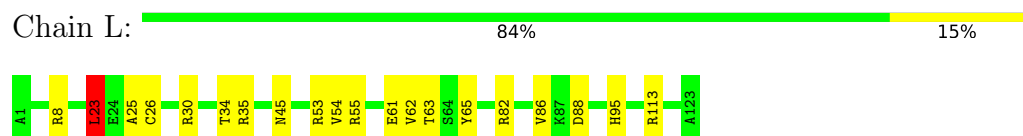
• Molecule 8: 30S ribosomal protein S6



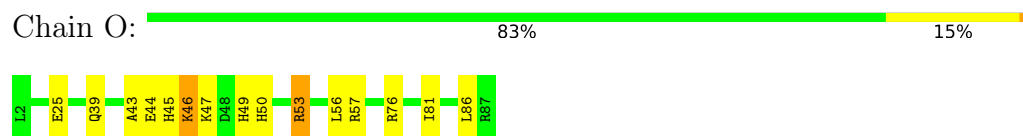
• Molecule 9: 30S ribosomal protein S8




• Molecule 10: 30S ribosomal protein S12



• Molecule 11: 30S ribosomal protein S15




• Molecule 12: 30S RIBOSOMAL PROTEIN bS16

Chain P:  81% 15%



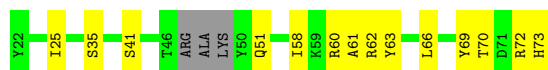
- Molecule 13: 30S ribosomal protein S17

Chain Q:  85% 15%




- Molecule 14: 30S ribosomal protein S18

Chain R:  67% 27% 6%




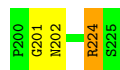
- Molecule 15: 30S ribosomal protein S20

Chain T:  78% 22%



- Molecule 16: 30S ribosomal protein S2

Chain B:  83% 17%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	423567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	C	0.30	0/1651	0.58	0/2225
10	L	0.39	0/969	0.72	1/1300 (0.1%)
11	O	0.29	0/706	0.59	0/944
12	P	0.41	0/639	0.71	2/859 (0.2%)
13	Q	0.40	0/650	0.62	0/871
14	R	0.31	0/411	0.58	0/552
15	T	0.31	0/665	0.53	0/881
16	B	0.31	0/1727	0.62	0/2328
2	J	0.29	0/796	0.64	1/1077 (0.1%)
3	N	0.28	0/785	0.62	1/1043 (0.1%)
4	S	0.28	0/609	0.56	0/822
5	A	0.62	0/32207	1.11	130/50237 (0.3%)
6	D	0.37	0/1665	0.63	0/2227
7	E	0.36	0/1101	0.62	0/1482
8	F	0.29	0/643	0.59	0/868
9	H	0.42	1/989 (0.1%)	0.70	2/1326 (0.2%)
All	All	0.55	1/46213 (0.0%)	1.00	137/69042 (0.2%)

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	C	0	2
10	L	0	1
16	B	0	1
2	J	0	2
6	D	0	1
9	H	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	78	SER	C-N	-5.83	1.20	1.34

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1158	C	N1-C2-O2	14.70	127.72	118.90
5	A	1158	C	C2-N1-C1'	12.75	132.83	118.80
5	A	1158	C	N3-C2-O2	-12.14	113.40	121.90
5	A	365	U	C2-N1-C1'	11.88	131.95	117.70
5	A	866	C	C6-N1-C2	-9.31	116.58	120.30
5	A	960	U	C2-N1-C1'	9.24	128.78	117.70
5	A	365	U	N1-C2-O2	8.93	129.05	122.80
5	A	1158	C	C6-N1-C2	-8.88	116.75	120.30
5	A	365	U	C6-N1-C1'	-8.85	108.81	121.20
5	A	1158	C	C6-N1-C1'	-8.69	110.37	120.80
3	N	50	LEU	CA-CB-CG	8.33	134.47	115.30
5	A	960	U	N1-C2-O2	8.06	128.45	122.80
5	A	1071	C	N1-C2-O2	8.06	123.74	118.90
5	A	481	G	N1-C6-O6	-8.06	115.06	119.90
5	A	1391	U	N1-C2-O2	7.90	128.33	122.80
5	A	322	C	C2-N1-C1'	7.89	127.47	118.80
5	A	754	C	N1-C2-O2	7.66	123.50	118.90
5	A	322	C	N1-C2-O2	7.66	123.50	118.90
5	A	599	C	N1-C2-O2	7.57	123.44	118.90
5	A	339	C	N1-C2-O2	7.46	123.38	118.90
5	A	960	U	N3-C2-O2	-7.46	116.98	122.20
5	A	372	C	P-O3'-C3'	7.34	128.51	119.70
5	A	855	U	N1-C2-O2	7.28	127.89	122.80
5	A	1391	U	N3-C2-O2	-7.07	117.25	122.20
5	A	866	C	C5-C6-N1	7.07	124.53	121.00
5	A	365	U	N3-C2-O2	-7.00	117.30	122.20
5	A	599	C	N3-C2-O2	-6.99	117.01	121.90
5	A	239	U	N1-C2-O2	6.90	127.63	122.80
5	A	1065	U	P-O3'-C3'	6.87	127.94	119.70
5	A	385	C	N1-C2-O2	6.83	123.00	118.90
5	A	322	C	C6-N1-C2	-6.81	117.58	120.30
5	A	1201	A	P-O3'-C3'	6.77	127.82	119.70
5	A	1391	U	C2-N1-C1'	6.75	125.80	117.70
5	A	401	C	N1-C2-O2	6.62	122.88	118.90
5	A	754	C	C2-N1-C1'	6.62	126.08	118.80
5	A	322	C	C5-C6-N1	6.61	124.31	121.00
5	A	484	G	P-O3'-C3'	6.60	127.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	A	P-O3'-C3'	6.59	127.61	119.70
5	A	462	G	N3-C4-C5	-6.54	125.33	128.60
5	A	1038	C	C5-C6-N1	6.54	124.27	121.00
5	A	1071	C	N3-C2-O2	-6.51	117.35	121.90
5	A	339	C	N3-C2-O2	-6.48	117.36	121.90
5	A	284	C	N1-C2-O2	6.47	122.78	118.90
5	A	51	A	P-O3'-C3'	6.46	127.46	119.70
5	A	462	G	C4-N9-C1'	6.42	134.84	126.50
5	A	372	C	OP2-P-O3'	6.39	119.25	105.20
5	A	1158	C	C5-C6-N1	6.34	124.17	121.00
5	A	239	U	N3-C2-O2	-6.33	117.77	122.20
5	A	599	C	C6-N1-C2	-6.31	117.78	120.30
5	A	54	C	N1-C2-O2	6.27	122.66	118.90
5	A	385	C	N3-C2-O2	-6.22	117.55	121.90
12	P	4	ILE	CG1-CB-CG2	-6.21	97.74	111.40
5	A	239	U	C2-N1-C1'	6.21	125.15	117.70
5	A	855	U	N3-C2-O2	-6.19	117.86	122.20
5	A	385	C	C2-N1-C1'	6.13	125.54	118.80
5	A	1195	C	N1-C2-O2	6.10	122.56	118.90
5	A	462	G	N3-C4-N9	6.10	129.66	126.00
5	A	365	U	C5-C6-N1	6.08	125.74	122.70
5	A	401	C	N3-C2-O2	-6.05	117.66	121.90
5	A	1038	C	C6-N1-C2	-6.04	117.88	120.30
5	A	1138	G	N3-C4-N9	6.04	129.62	126.00
5	A	823	C	C6-N1-C2	-6.02	117.89	120.30
5	A	1322	C	C2-N1-C1'	6.02	125.42	118.80
5	A	51	A	OP2-P-O3'	6.01	118.43	105.20
5	A	672	U	N1-C2-O2	6.01	127.01	122.80
5	A	284	C	N3-C2-O2	-5.98	117.71	121.90
5	A	322	C	N3-C2-O2	-5.98	117.72	121.90
5	A	355	C	C6-N1-C2	-5.97	117.91	120.30
5	A	328	C	P-O3'-C3'	5.97	126.87	119.70
5	A	929	G	P-O3'-C3'	5.97	126.87	119.70
5	A	960	U	C6-N1-C1'	-5.97	112.84	121.20
5	A	1138	G	C4-N9-C1'	5.93	134.21	126.50
5	A	1071	C	C2-N1-C1'	5.90	125.29	118.80
5	A	328	C	OP2-P-O3'	5.86	118.10	105.20
5	A	1138	G	N3-C4-C5	-5.83	125.68	128.60
9	H	120	LEU	CA-CB-CG	5.83	128.72	115.30
5	A	481	G	C5-C6-O6	5.83	132.10	128.60
10	L	23	LEU	CA-CB-CG	5.80	128.64	115.30
5	A	180	U	N3-C2-O2	-5.79	118.15	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	244	U	O5'-P-OP2	5.72	117.56	110.70
5	A	295	C	C6-N1-C2	-5.72	118.01	120.30
5	A	1300	G	P-O3'-C3'	5.70	126.55	119.70
5	A	401	C	C2-N1-C1'	5.70	125.07	118.80
5	A	295	C	N1-C2-O2	5.67	122.30	118.90
5	A	855	U	C2-N1-C1'	5.67	124.50	117.70
9	H	78	SER	C-N-CA	5.63	135.78	121.70
5	A	500	G	C4-N9-C1'	5.62	133.81	126.50
5	A	614	C	C6-N1-C2	-5.62	118.05	120.30
5	A	868	C	N3-C2-O2	-5.60	117.98	121.90
5	A	882	C	C6-N1-C2	-5.59	118.06	120.30
5	A	295	C	N3-C2-O2	-5.58	117.99	121.90
5	A	328	C	N1-C2-O2	5.57	122.24	118.90
12	P	42	ILE	CG1-CB-CG2	-5.55	99.19	111.40
5	A	413	G	N3-C4-N9	5.52	129.31	126.00
5	A	385	C	C6-N1-C2	-5.49	118.10	120.30
5	A	283	U	N3-C2-O2	-5.47	118.37	122.20
5	A	758	C	C5-C6-N1	5.47	123.73	121.00
5	A	514	C	C6-N1-C2	-5.47	118.11	120.30
5	A	243	A	P-O3'-C3'	5.41	126.19	119.70
5	A	295	C	C2-N1-C1'	5.41	124.75	118.80
5	A	854	U	N1-C2-O2	5.40	126.58	122.80
5	A	180	U	N1-C2-O2	5.39	126.58	122.80
5	A	1282	C	C6-N1-C2	-5.39	118.14	120.30
5	A	599	C	C2-N1-C1'	5.36	124.70	118.80
5	A	868	C	N1-C2-O2	5.36	122.11	118.90
5	A	156	C	N1-C2-O2	5.33	122.10	118.90
5	A	486	U	N3-C2-O2	-5.32	118.47	122.20
5	A	672	U	N3-C2-O2	-5.32	118.48	122.20
5	A	754	C	C6-N1-C1'	-5.31	114.43	120.80
5	A	672	U	C2-N1-C1'	5.30	124.07	117.70
5	A	346	G	N3-C4-N9	5.29	129.17	126.00
5	A	960	U	C5-C6-N1	5.23	125.31	122.70
5	A	500	G	C8-N9-C1'	-5.22	120.21	127.00
5	A	582	C	N1-C2-O2	5.22	122.03	118.90
5	A	209	U	N1-C2-O2	5.22	126.45	122.80
5	A	678	U	C5-C6-N1	5.21	125.30	122.70
5	A	584	G	C4-N9-C1'	5.19	133.24	126.50
5	A	108	G	C4-C5-N7	5.18	112.87	110.80
5	A	43	C	C6-N1-C2	-5.18	118.23	120.30
5	A	54	C	N3-C2-O2	-5.18	118.27	121.90
5	A	20	U	N3-C2-O2	-5.18	118.58	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	283	U	N1-C2-O2	5.18	126.42	122.80
5	A	99	C	C6-N1-C2	-5.17	118.23	120.30
5	A	180	U	C2-N1-C1'	5.16	123.89	117.70
5	A	222	C	N1-C2-O2	5.15	121.99	118.90
5	A	1369	C	N1-C2-O2	5.14	121.99	118.90
2	J	42	LEU	CA-CB-CG	5.13	127.11	115.30
5	A	530	G	C4-N9-C1'	5.10	133.13	126.50
5	A	1367	C	C6-N1-C2	-5.10	118.26	120.30
5	A	1138	G	C8-N9-C1'	-5.09	120.39	127.00
5	A	563	A	C4-N9-C1'	5.06	135.41	126.30
5	A	1056	U	N1-C2-O2	5.05	126.34	122.80
5	A	92	U	N1-C2-O2	5.05	126.34	122.80
5	A	810	C	N1-C2-O2	5.05	121.93	118.90
5	A	1125	U	C2-N1-C1'	5.05	123.76	117.70
5	A	751	U	N1-C2-O2	5.04	126.33	122.80
5	A	462	G	C8-N9-C1'	-5.04	120.45	127.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	B	129	THR	Peptide
1	C	166	TRP	Peptide
1	C	24	ASN	Peptide
6	D	176	LYS	Peptide
9	H	111	THR	Peptide
9	H	3	GLN	Peptide
2	J	14	ASP	Peptide
2	J	41	PRO	Peptide
10	L	23	LEU	Peptide

## 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	C	1624	0	1699	28	0
2	J	786	0	828	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	774	0	827	17	0
4	S	594	0	610	16	0
5	A	28767	0	14485	267	0
6	D	1643	0	1710	28	0
7	E	1089	0	1128	19	0
8	F	630	0	626	7	0
9	H	979	0	1033	18	0
10	L	955	0	1019	15	0
11	O	698	0	721	12	0
12	P	629	0	643	10	0
13	Q	641	0	682	7	0
14	R	405	0	425	10	0
15	T	659	0	703	15	0
16	B	1696	0	1723	22	0
17	A	1	0	0	0	0
All	All	42570	0	28862	431	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 8.

All (431) 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)
5:A:1349:A:H62	5:A:1373:G:H21	1.36	0.71
5:A:674:G:H1	5:A:715:A:H61	1.38	0.71
5:A:993:G:H2'	5:A:995:C:H41	1.58	0.67
5:A:659:U:H3	5:A:746:A:H61	1.44	0.66
5:A:928:G:H1	5:A:1389:C:H42	1.42	0.66
5:A:988:G:H4'	5:A:1014:A:H61	1.59	0.66
5:A:1097:C:HO2'	5:A:1169:A:HO2'	1.43	0.66
5:A:551:U:O2'	10:L:82:ARG:NH1	2.29	0.66
1:C:149:LYS:HB3	1:C:200:TRP:HB2	1.78	0.65
12:P:14:ARG:HE	12:P:42:ILE:HD13	1.61	0.65
4:S:65:MET:HA	4:S:68:HIS:HB3	1.77	0.65
6:D:161:ALA:HA	6:D:164:ARG:HD3	1.79	0.65
5:A:667:G:O6	5:A:739:C:N4	2.30	0.64
5:A:655:A:H61	5:A:751:U:H3	1.46	0.63
5:A:542:G:OP1	6:D:9:LYS:NZ	2.32	0.63
5:A:978:A:OP2	5:A:1362:A:N6	2.32	0.63
5:A:617:G:H1	5:A:623:C:H42	1.47	0.62
1:C:34:SER:OG	1:C:58:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1120:C:H42	5:A:1153:G:H1	1.45	0.62
6:D:61:ARG:HH21	6:D:67:LEU:HA	1.64	0.62
5:A:1089:G:N2	5:A:1097:C:N3	2.47	0.61
16:B:14:HIS:HB2	16:B:202:ASN:HD22	1.66	0.61
5:A:1121:U:H3	5:A:1152:A:H61	1.48	0.61
5:A:1064:G:O2'	5:A:1190:G:N2	2.34	0.61
14:R:35:SER:HB2	14:R:72:ARG:HH12	1.65	0.60
5:A:1103:C:H4'	16:B:96:LEU:HD22	1.83	0.60
5:A:664:G:H22	5:A:741:G:H1	1.49	0.60
5:A:1178:G:N2	5:A:1181:G:OP2	2.34	0.60
5:A:111:G:O6	5:A:330:C:N4	2.33	0.60
5:A:178:C:H2'	5:A:179:A:H8	1.66	0.60
5:A:677:U:H3	5:A:713:G:H1	1.50	0.60
5:A:916:U:H2'	5:A:917:G:H8	1.67	0.59
5:A:363:A:N6	10:L:26:CYS:SG	2.75	0.59
1:C:55:VAL:HB	1:C:66:THR:HB	1.85	0.59
5:A:987:G:H21	5:A:1014:A:H2	1.50	0.59
9:H:38:VAL:HG22	9:H:110:MET:HG3	1.84	0.59
4:S:52:ASN:O	5:A:958:A:N6	2.35	0.59
16:B:65:LYS:HB2	16:B:158:ASP:H	1.68	0.59
6:D:171:GLU:HB2	6:D:180:THR:HB	1.85	0.58
1:C:149:LYS:HB2	1:C:172:VAL:HG21	1.85	0.58
2:J:39:PRO:HB3	2:J:72:ARG:HH21	1.68	0.58
10:L:53:ARG:HA	10:L:63:THR:HA	1.85	0.58
5:A:767:A:N6	5:A:813:U:O2	2.36	0.58
16:B:31:PHE:HB2	16:B:41:ASN:HB2	1.84	0.58
16:B:87:ASP:HB3	16:B:224:ARG:HH22	1.69	0.58
5:A:178:C:OP2	15:T:59:ARG:NH1	2.36	0.58
5:A:985:C:H42	5:A:1220:G:H1	1.50	0.58
5:A:373:A:H1'	5:A:481:G:H1'	1.85	0.58
5:A:185:U:O2	15:T:75:LYS:NZ	2.36	0.58
5:A:197:A:O2'	5:A:220:G:N2	2.36	0.58
5:A:49:U:O2'	5:A:361:G:N2	2.37	0.58
5:A:486:U:H2'	5:A:487:A:H8	1.68	0.58
12:P:11:ALA:HB3	12:P:14:ARG:HB2	1.84	0.57
5:A:1097:C:H5'	16:B:138:ARG:HD3	1.86	0.57
5:A:977:A:O2'	5:A:1223:C:N4	2.37	0.57
3:N:100:TRP:OXT	5:A:1186:G:N2	2.36	0.57
5:A:344:A:OP2	5:A:345:C:N4	2.37	0.57
5:A:491:G:OP1	6:D:147:LYS:NZ	2.38	0.57
3:N:99:SER:O	5:A:1114:C:O2'	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:517:G:N1	5:A:533:A:OP2	2.35	0.57
5:A:764:C:OP2	5:A:765:G:N2	2.38	0.57
5:A:822:U:H3	5:A:878:A:H61	1.52	0.57
4:S:12:LEU:HA	4:S:15:LEU:HB3	1.87	0.57
5:A:998:C:O2	5:A:1043:G:N2	2.38	0.57
5:A:939:G:O2'	5:A:1375:A:N3	2.37	0.57
5:A:1071:C:H42	5:A:1104:G:H1	1.53	0.57
5:A:662:U:O2'	5:A:836:G:OP1	2.22	0.57
1:C:33:ASP:OD1	3:N:65:GLN:NE2	2.36	0.57
5:A:108:G:H5'	5:A:109:A:H5''	1.86	0.57
5:A:411:A:OP1	6:D:25:ARG:NH2	2.37	0.57
6:D:149:LYS:NZ	6:D:177:MET:SD	2.77	0.56
7:E:77:ASN:ND2	7:E:100:GLU:OE2	2.38	0.56
5:A:263:A:OP1	15:T:73:ARG:NH1	2.38	0.56
6:D:10:LEU:HD21	6:D:62:ARG:HD3	1.85	0.56
5:A:16:A:OP1	7:E:19:ARG:NH2	2.38	0.56
9:H:83:ARG:NH1	9:H:123:GLU:OE2	2.38	0.56
9:H:6:ILE:HD12	9:H:35:ILE:HD11	1.85	0.56
6:D:14:GLU:OE2	6:D:55:ARG:NH1	2.38	0.56
2:J:8:ILE:HB	2:J:74:VAL:HB	1.88	0.56
14:R:41:SER:HB2	14:R:51:GLN:HG2	1.88	0.56
5:A:1305:G:N1	5:A:1331:G:N3	2.53	0.56
3:N:12:ARG:NH1	5:A:980:C:O3'	2.39	0.56
5:A:1118:U:H3	5:A:1155:A:H61	1.54	0.55
5:A:570:G:N2	5:A:867:G:O2'	2.38	0.55
10:L:86:VAL:HG12	10:L:88:ASP:H	1.71	0.55
4:S:49:ALA:HA	4:S:58:PRO:HA	1.89	0.55
10:L:34:THR:HG22	10:L:35:ARG:HG2	1.87	0.55
11:O:25:GLU:HG3	11:O:76:ARG:HH21	1.72	0.55
5:A:18:C:H42	5:A:917:G:H1	1.53	0.55
6:D:104:MET:HG2	6:D:170:LEU:HD13	1.89	0.55
5:A:1347:G:N2	5:A:1374:A:OP2	2.39	0.55
6:D:25:ARG:HE	6:D:30:LYS:HD2	1.71	0.55
5:A:919:A:O2'	5:A:1080:A:N1	2.39	0.55
5:A:458:U:H3	5:A:474:G:H1	1.54	0.54
5:A:952:U:O2'	5:A:969:A:N1	2.41	0.54
12:P:4:ILE:HG23	12:P:21:VAL:HG22	1.88	0.54
9:H:5:PRO:O	9:H:32:LYS:NZ	2.33	0.54
9:H:14:ARG:NH1	9:H:74:ILE:O	2.41	0.54
6:D:12:ARG:NH1	6:D:31:CYS:O	2.41	0.54
13:Q:19:SER:OG	13:Q:70:LYS:NZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:977:A:H8	5:A:1362:A:H61	1.55	0.54
5:A:764:C:N4	5:A:812:G:O6	2.41	0.54
5:A:21:G:H21	5:A:914:A:H62	1.56	0.54
5:A:1072:G:H1	5:A:1103:C:H42	1.56	0.54
2:J:43:PRO:HG2	2:J:71:LEU:HD12	1.89	0.54
5:A:736:C:OP1	14:R:60:ARG:NH2	2.41	0.54
14:R:25:ILE:HB	14:R:66:LEU:HD13	1.90	0.54
5:A:1166:G:N1	5:A:1169:A:OP2	2.40	0.53
5:A:522:C:OP2	10:L:65:TYR:OH	2.26	0.53
5:A:56:U:O4	5:A:357:G:N2	2.42	0.53
5:A:667:G:O2'	11:O:50:HIS:ND1	2.41	0.53
5:A:1098:C:OP1	16:B:142:LYS:NZ	2.41	0.53
5:A:1316:G:N2	5:A:1319:A:OP2	2.37	0.53
1:C:27:GLU:O	1:C:31:ASN:ND2	2.41	0.53
15:T:58:ASP:HA	15:T:61:ALA:HB3	1.90	0.53
5:A:1266:G:O2'	5:A:1269:A:N6	2.41	0.53
5:A:1310:G:H1	5:A:1328:C:H42	1.56	0.53
5:A:1289:A:N1	5:A:1371:G:O2'	2.40	0.53
11:O:81:ILE:HG22	11:O:86:LEU:HD12	1.88	0.53
5:A:62:U:OP1	5:A:385:C:O2'	2.26	0.53
7:E:156:ARG:NH2	9:H:98:LEU:O	2.42	0.53
1:C:96:VAL:HG12	1:C:98:ALA:HB2	1.91	0.53
2:J:87:LEU:HD12	2:J:90:LEU:HD12	1.90	0.53
5:A:528:C:N4	10:L:45:ASN:OD1	2.41	0.52
3:N:63:CYS:HB3	3:N:68:ARG:H	1.73	0.52
3:N:9:GLU:OE1	3:N:60:ARG:NH2	2.41	0.52
5:A:1291:U:H2'	5:A:1292:G:H8	1.74	0.52
5:A:411:A:H2	5:A:430:A:H62	1.57	0.52
5:A:67:C:O2'	5:A:171:A:N3	2.43	0.52
5:A:176:C:OP1	15:T:23:ARG:NH1	2.42	0.52
5:A:773:G:H22	5:A:806:C:H42	1.58	0.52
5:A:1075:U:O2'	16:B:173:LYS:NZ	2.42	0.52
9:H:88:LYS:HE3	9:H:119:GLY:HA2	1.91	0.52
4:S:15:LEU:HA	4:S:18:VAL:HG12	1.91	0.52
5:A:1363:A:O2'	5:A:1365:G:N7	2.39	0.52
5:A:598:U:H2'	5:A:599:C:H6	1.74	0.52
5:A:734:G:N2	14:R:63:TYR:OH	2.42	0.52
5:A:669:G:OP1	11:O:47:LYS:NZ	2.38	0.52
8:F:1:MET:HG2	8:F:67:PRO:HB3	1.91	0.52
5:A:962:C:H2'	5:A:963:G:H8	1.75	0.52
4:S:31:ARG:HE	4:S:56:HIS:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1241:G:H1	5:A:1296:C:H1'	1.75	0.51
5:A:858:G:H3'	5:A:869:G:H1	1.74	0.51
5:A:842:U:O2'	5:A:846:G:N1	2.43	0.51
16:B:11:ALA:HB3	16:B:42:LEU:HD21	1.92	0.51
5:A:854:U:H3'	5:A:871:U:H3	1.76	0.51
1:C:153:SER:HB2	1:C:196:GLY:H	1.74	0.51
5:A:1305:G:O2'	5:A:1332:A:N6	2.44	0.51
7:E:110:MET:HB3	7:E:139:THR:HG21	1.92	0.51
2:J:36:VAL:HA	2:J:76:ILE:HG22	1.93	0.51
5:A:1130:A:N6	5:A:1144:G:O2'	2.42	0.51
5:A:184:G:N2	5:A:194:C:N3	2.58	0.51
5:A:501:C:OP2	10:L:113:ARG:NH2	2.44	0.51
5:A:296:U:H2'	5:A:297:G:H8	1.76	0.51
7:E:93:VAL:HG11	7:E:139:THR:HG22	1.92	0.51
5:A:1015:G:N2	5:A:1218:C:O2	2.44	0.50
5:A:770:C:H2'	5:A:771:G:H8	1.75	0.50
16:B:75:ALA:HA	16:B:78:ALA:HB3	1.93	0.50
5:A:505:G:H2'	5:A:506:G:H8	1.76	0.50
5:A:855:U:OP2	5:A:871:U:N3	2.38	0.50
2:J:24:GLU:O	2:J:28:THR:OG1	2.29	0.50
11:O:45:HIS:O	11:O:47:LYS:N	2.44	0.50
11:O:53:ARG:O	11:O:57:ARG:N	2.43	0.50
5:A:618:C:H1'	12:P:14:ARG:HH12	1.77	0.50
5:A:1249:C:O2	5:A:1288:A:N6	2.43	0.50
5:A:571:U:O4	5:A:865:A:N6	2.42	0.50
1:C:149:LYS:HG3	1:C:168:ARG:HG2	1.93	0.50
5:A:204:G:N1	5:A:465:A:OP1	2.44	0.50
4:S:57:VAL:HG23	4:S:74:ALA:HB1	1.94	0.50
5:A:393:A:H2'	5:A:394:G:H8	1.76	0.50
5:A:831:A:OP1	16:B:20:ARG:NH1	2.43	0.50
5:A:826:C:O5'	9:H:12:ARG:NH1	2.45	0.50
5:A:1055:A:N1	5:A:1205:U:O2'	2.45	0.49
1:C:117:ASP:OD1	1:C:120:THR:OG1	2.29	0.49
5:A:384:G:H2'	5:A:385:C:H6	1.78	0.49
14:R:70:THR:HG23	14:R:73:HIS:H	1.77	0.49
2:J:62:ARG:NH2	5:A:1190:G:N7	2.44	0.49
5:A:986:U:H2'	5:A:987:G:C8	2.48	0.49
5:A:619:U:N3	6:D:130:ASN:OD1	2.41	0.49
5:A:542:G:O3'	6:D:13:ARG:NH2	2.45	0.49
5:A:1268:G:N3	5:A:1326:U:O2'	2.44	0.49
5:A:501:C:H2'	5:A:502:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:201:GLU:OE2	7:E:104:ILE:N	2.44	0.49
5:A:1166:G:O2'	5:A:1169:A:N6	2.46	0.49
5:A:448:A:H62	5:A:486:U:H3	1.59	0.49
5:A:408:A:O2'	6:D:153:ARG:NH2	2.46	0.49
5:A:730:G:N2	5:A:766:A:OP1	2.41	0.48
5:A:937:A:H2'	5:A:938:A:H8	1.77	0.48
3:N:15:LEU:HA	3:N:18:LYS:HB2	1.93	0.48
5:A:1301:U:O2'	5:A:1303:C:OP2	2.31	0.48
5:A:52:C:H2'	5:A:53:A:H8	1.78	0.48
5:A:940:C:O2	5:A:1343:G:N2	2.30	0.48
16:B:119:GLN:NE2	16:B:124:THR:O	2.46	0.48
1:C:81:GLU:OE2	1:C:85:LYS:NZ	2.38	0.48
6:D:128:VAL:HG22	6:D:145:ARG:HD3	1.96	0.48
5:A:613:C:OP2	6:D:80:ARG:NH1	2.46	0.48
5:A:427:U:H3'	5:A:428:G:H2'	1.95	0.48
5:A:866:C:C4	5:A:867:G:H1'	2.49	0.48
7:E:14:LEU:HA	7:E:36:THR:HG22	1.96	0.48
2:J:64:GLN:HG3	3:N:98:ALA:HB3	1.95	0.48
5:A:994:A:H61	5:A:1046:A:H2'	1.78	0.48
5:A:662:U:H2'	5:A:663:A:C8	2.48	0.48
5:A:718:A:N1	14:R:62:ARG:NH2	2.57	0.48
5:A:897:C:H42	5:A:902:G:H1	1.62	0.48
16:B:128:LEU:HD12	16:B:132:GLU:HG2	1.96	0.48
4:S:35:ARG:NH2	5:A:1321:U:O2	2.47	0.48
5:A:209:U:H5''	5:A:210:C:H5	1.79	0.47
5:A:615:G:H2'	5:A:616:G:H8	1.79	0.47
5:A:823:C:N4	5:A:824:G:O6	2.47	0.47
8:F:11:HIS:HE1	8:F:13:ASP:HB2	1.79	0.47
5:A:390:U:O5'	12:P:28:ARG:NH1	2.47	0.47
5:A:986:U:H2'	5:A:987:G:H8	1.79	0.47
5:A:59:A:H3'	5:A:331:G:H22	1.78	0.47
5:A:58:C:O2'	5:A:388:G:N7	2.47	0.47
7:E:152:VAL:HG21	9:H:98:LEU:HD23	1.96	0.47
5:A:1185:G:H2'	5:A:1186:G:H8	1.79	0.47
5:A:157:U:H3	5:A:164:G:H1	1.63	0.47
4:S:77:ARG:NH1	5:A:1223:C:OP1	2.47	0.47
1:C:9:ILE:HG23	1:C:10:ARG:HG3	1.94	0.47
5:A:826:C:H4'	9:H:12:ARG:HG2	1.95	0.47
5:A:1046:A:N6	5:A:1212:U:OP2	2.48	0.47
5:A:1126:U:N3	5:A:1280:A:OP1	2.42	0.47
16:B:65:LYS:H	16:B:158:ASP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:391:G:OP1	12:P:8:ARG:NH1	2.47	0.47
5:A:1376:U:H2'	5:A:1377:A:H8	1.80	0.47
6:D:84:ASN:HB3	6:D:87:GLU:HB3	1.96	0.47
5:A:1100:C:C4	5:A:1102:A:H5'	2.50	0.47
5:A:1181:G:H1'	5:A:1182:G:C4	2.50	0.47
5:A:1241:G:H2'	5:A:1242:G:C8	2.50	0.47
5:A:642:A:C5	9:H:106:SER:HA	2.50	0.47
5:A:1209:C:O2	5:A:1214:C:N4	2.38	0.47
5:A:243:A:N6	5:A:283:U:O4	2.47	0.47
5:A:96:U:H2'	5:A:97:G:H8	1.80	0.47
5:A:1355:G:O6	5:A:1366:C:N4	2.48	0.47
5:A:121:U:N3	5:A:235:C:OP2	2.48	0.47
7:E:102:THR:O	7:E:121:ASN:ND2	2.41	0.47
7:E:73:VAL:HG11	7:E:143:LEU:HB3	1.96	0.47
3:N:81:ILE:HD12	3:N:82:LYS:HG2	1.97	0.47
5:A:462:G:H22	5:A:470:C:H42	1.64	0.47
13:Q:4:ILE:HG13	13:Q:5:ARG:H	1.80	0.47
5:A:130:A:H5'	13:Q:64:ARG:HD3	1.97	0.46
5:A:1238:A:H5'	5:A:1336:C:H41	1.80	0.46
6:D:8:LEU:HD21	6:D:21:LYS:HB2	1.97	0.46
7:E:82:HIS:HE2	7:E:147:ASN:H	1.61	0.46
2:J:92:LEU:HA	2:J:93:ALA:HA	1.56	0.46
11:O:44:GLU:HA	11:O:46:LYS:HE3	1.97	0.46
14:R:25:ILE:HD12	14:R:66:LEU:HD22	1.97	0.46
5:A:1243:C:N4	5:A:1244:G:O6	2.48	0.46
5:A:162:A:C5	5:A:163:C:H1'	2.50	0.46
5:A:1158:C:H5''	16:B:131:LYS:HD3	1.97	0.46
2:J:7:ARG:HB2	2:J:101:SER:HB3	1.97	0.46
5:A:104:G:O6	15:T:8:LYS:NZ	2.42	0.46
5:A:1297:G:N2	5:A:1298:U:O4	2.47	0.46
8:F:32:ALA:HB2	8:F:70:VAL:HG21	1.98	0.46
5:A:373:A:H2'	5:A:481:G:H21	1.81	0.46
10:L:34:THR:O	10:L:35:ARG:NE	2.44	0.46
5:A:343:U:O2'	5:A:346:G:O6	2.24	0.46
5:A:579:A:O3'	11:O:53:ARG:NH2	2.49	0.46
5:A:868:C:H3'	5:A:869:G:H8	1.81	0.46
1:C:152:VAL:H	1:C:165:GLU:HB2	1.80	0.46
9:H:26:MET:SD	9:H:26:MET:N	2.89	0.46
4:S:17:LYS:HE3	4:S:32:THR:HA	1.96	0.46
5:A:1305:G:O2'	5:A:1306:A:O4'	2.29	0.46
16:B:57:ASN:O	16:B:61:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:186:C:O2'	15:T:75:LYS:O	2.32	0.46
16:B:130:LYS:HA	16:B:133:ALA:HB3	1.98	0.46
1:C:39:ARG:HH11	3:N:91:GLU:HG2	1.81	0.46
1:C:19:SER:HB2	1:C:39:ARG:HH22	1.80	0.46
13:Q:57:VAL:H	13:Q:79:GLU:HB3	1.81	0.46
5:A:96:U:H2'	5:A:97:G:C8	2.51	0.45
4:S:52:ASN:HB2	4:S:76:THR:HA	1.98	0.45
5:A:264:C:H4'	13:Q:64:ARG:HD2	1.97	0.45
15:T:43:LYS:NZ	15:T:82:ILE:O	2.40	0.45
5:A:1185:G:H2'	5:A:1186:G:C8	2.51	0.45
5:A:651:C:N4	5:A:752:G:O2'	2.49	0.45
16:B:86:CYS:O	16:B:88:GLN:NE2	2.50	0.45
6:D:137:SER:OG	6:D:140:ASP:OD2	2.35	0.45
1:C:20:THR:HA	3:N:93:PRO:HB3	1.98	0.45
5:A:410:G:H5''	6:D:25:ARG:HH22	1.81	0.45
5:A:438:U:O2'	5:A:493:A:N6	2.47	0.45
5:A:563:A:H61	5:A:884:U:H3	1.65	0.45
5:A:592:G:H1	5:A:647:C:H42	1.65	0.45
5:A:842:U:H3'	5:A:843:U:H4'	1.98	0.45
13:Q:53:GLY:N	13:Q:56:ASP:OD2	2.39	0.45
4:S:51:HIS:ND1	5:A:1220:G:O2'	2.39	0.45
6:D:169:TRP:CD2	6:D:185:PRO:HB3	2.52	0.45
9:H:29:SER:H	9:H:32:LYS:HD2	1.82	0.45
10:L:23:LEU:HB3	10:L:25:ALA:H	1.82	0.45
15:T:57:VAL:HG13	15:T:71:ALA:HB1	1.99	0.45
5:A:1094:G:O2'	5:A:1108:G:N2	2.46	0.45
5:A:673:A:N3	5:A:674:G:N2	2.65	0.45
5:A:925:G:N2	5:A:927:G:O4'	2.50	0.45
4:S:36:ARG:HG2	5:A:1320:C:H41	1.81	0.45
5:A:236:A:H2'	5:A:237:G:H8	1.82	0.45
5:A:671:G:O2'	8:F:79:ARG:NH1	2.50	0.45
5:A:1162:C:H2'	5:A:1163:A:C8	2.52	0.44
1:C:160:GLU:OE2	5:A:1206:G:N2	2.51	0.44
5:A:539:A:H2'	5:A:540:G:H8	1.83	0.44
5:A:1004:A:OP1	5:A:1024:G:N1	2.50	0.44
5:A:623:C:H2'	5:A:624:C:H6	1.83	0.44
16:B:118:THR:HA	16:B:121:GLN:HE21	1.81	0.44
1:C:186:SER:OG	1:C:187:GLU:N	2.49	0.44
6:D:189:ASP:N	6:D:189:ASP:OD1	2.48	0.44
3:N:50:LEU:HA	4:S:12:LEU:HD22	1.99	0.44
5:A:995:C:H2'	5:A:996:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1328:C:H2'	5:A:1329:A:C8	2.53	0.44
5:A:712:A:C6	5:A:713:G:H1'	2.53	0.44
5:A:881:G:OP1	10:L:8:ARG:NH1	2.46	0.44
7:E:156:ARG:O	9:H:63:LYS:NZ	2.50	0.44
5:A:825:A:H2	9:H:11:THR:HG21	1.82	0.44
3:N:63:CYS:SG	3:N:64:ARG:N	2.90	0.44
5:A:1020:G:H2'	5:A:1021:A:C8	2.53	0.44
5:A:1278:G:H1'	5:A:1279:G:H21	1.80	0.44
5:A:455:G:H1	5:A:477:C:H42	1.65	0.44
5:A:1073:U:H3	5:A:1102:A:H61	1.65	0.44
5:A:833:G:H1	5:A:853:C:H42	1.66	0.43
8:F:26:THR:HG23	8:F:29:ILE:HD12	1.99	0.43
5:A:1099:G:N1	5:A:1100:C:O2	2.52	0.43
5:A:1250:A:H61	5:A:1354:U:H4'	1.82	0.43
5:A:31:G:H8	5:A:31:G:H5''	1.83	0.43
5:A:360:G:H2'	5:A:361:G:C8	2.53	0.43
5:A:539:A:H2'	5:A:540:G:C8	2.52	0.43
5:A:974:A:H4'	5:A:975:A:H3'	1.99	0.43
5:A:1305:G:H1	5:A:1331:G:H1'	1.84	0.43
5:A:141:G:H2'	5:A:142:G:H8	1.83	0.43
5:A:741:G:H2'	5:A:742:G:H8	1.83	0.43
16:B:199:ILE:HG22	16:B:201:GLY:H	1.84	0.43
6:D:24:VAL:HG12	6:D:25:ARG:H	1.82	0.43
5:A:1125:U:H2'	5:A:1126:U:H2'	1.99	0.43
10:L:54:VAL:N	10:L:62:VAL:O	2.46	0.43
15:T:6:ALA:O	15:T:10:ALA:N	2.42	0.43
5:A:202:G:H21	5:A:465:A:H61	1.67	0.43
6:D:32:LYS:HB3	6:D:35:GLN:HB2	2.01	0.43
10:L:82:ARG:HB3	10:L:95:HIS:HB3	1.99	0.43
7:E:79:THR:HB	7:E:121:ASN:HB2	2.01	0.43
4:S:22:VAL:HG22	4:S:46:LEU:HG	2.01	0.43
5:A:1037:C:H2'	5:A:1038:C:H6	1.84	0.43
5:A:105:G:O6	15:T:8:LYS:NZ	2.37	0.43
5:A:392:C:H4'	12:P:13:LYS:HE3	2.01	0.43
5:A:404:G:O2'	5:A:439:U:N3	2.43	0.43
5:A:865:A:N3	5:A:918:A:O2'	2.49	0.43
12:P:20:VAL:HG13	12:P:32:PHE:HB3	2.00	0.43
5:A:1070:U:H2'	5:A:1071:C:H6	1.83	0.43
10:L:55:ARG:HA	10:L:61:GLU:HG2	2.01	0.43
5:A:824:G:H2'	5:A:825:A:C8	2.54	0.42
2:J:7:ARG:NH2	2:J:102:LEU:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:536:C:H2'	5:A:537:G:H8	1.84	0.42
5:A:868:C:H3'	5:A:869:G:C8	2.54	0.42
3:N:2:LYS:HD3	5:A:1049:U:H2'	2.02	0.42
5:A:541:G:H2'	5:A:542:G:H8	1.84	0.42
1:C:70:ALA:HA	1:C:104:GLU:HG3	2.01	0.42
3:N:81:ILE:H	3:N:81:ILE:HG13	1.56	0.42
5:A:200:G:O2'	5:A:381:C:N4	2.53	0.42
5:A:74:A:H2'	5:A:75:G:C8	2.54	0.42
5:A:764:C:H4'	11:O:49:HIS:HB3	2.00	0.42
5:A:1110:A:N7	5:A:1111:A:N6	2.68	0.42
5:A:891:U:H2'	5:A:892:A:H8	1.83	0.42
3:N:5:MET:O	3:N:9:GLU:N	2.53	0.42
5:A:588:G:H1	5:A:651:C:H42	1.68	0.42
16:B:33:ALA:HA	16:B:38:HIS:HA	2.01	0.42
6:D:9:LYS:HE3	6:D:9:LYS:HB2	1.80	0.42
8:F:25:TYR:HB3	8:F:74:LEU:HD11	2.01	0.42
2:J:15:HIS:CD2	5:A:1152:A:H4'	2.55	0.42
5:A:1096:C:H2'	5:A:1097:C:C6	2.53	0.42
14:R:58:ILE:HA	14:R:61:ALA:HB2	2.01	0.42
1:C:15:LYS:HD2	1:C:16:PRO:HD2	2.02	0.42
11:O:39:GLN:O	11:O:43:ALA:N	2.53	0.42
15:T:23:ARG:HB3	15:T:60:GLN:HE22	1.84	0.42
5:A:1144:G:H21	5:A:1146:A:H62	1.68	0.41
5:A:229:U:H2'	5:A:230:G:H8	1.84	0.41
2:J:40:ILE:HD12	2:J:42:LEU:HD11	2.02	0.41
5:A:1040:U:H2'	5:A:1041:G:C8	2.55	0.41
5:A:296:U:H2'	5:A:297:G:C8	2.54	0.41
5:A:352:C:H42	5:A:357:G:H22	1.68	0.41
5:A:639:G:H2'	5:A:640:A:H8	1.85	0.41
1:C:39:ARG:HG3	1:C:54:ILE:HD12	2.02	0.41
7:E:20:VAL:O	7:E:31:SER:N	2.54	0.41
5:A:1261:A:N6	5:A:1274:A:O2'	2.45	0.41
5:A:579:A:N3	5:A:763:G:N2	2.69	0.41
5:A:9:G:H5'	7:E:107:GLY:HA3	2.02	0.41
5:A:362:G:H5''	10:L:30:ARG:HH12	1.85	0.41
12:P:23:ASP:OD1	12:P:24:SER:N	2.53	0.41
5:A:10:A:H2'	5:A:11:G:H8	1.85	0.41
5:A:1250:A:H2	5:A:1353:G:H21	1.67	0.41
1:C:10:ARG:NH2	1:C:174:LEU:O	2.41	0.41
3:N:52:ARG:NH1	5:A:1220:G:OP2	2.52	0.41
5:A:222:C:H2'	5:A:223:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:370:C:H42	5:A:391:G:H1	1.69	0.41
5:A:398:U:H2'	5:A:399:G:H8	1.85	0.41
7:E:35:LEU:HD11	7:E:133:ILE:HG12	2.03	0.41
5:A:579:A:O2'	11:O:53:ARG:NH2	2.53	0.41
4:S:77:ARG:NH2	5:A:1322:C:OP1	2.53	0.41
5:A:114:U:H1'	5:A:353:A:H1'	2.02	0.41
1:C:107:LYS:HB3	1:C:110:LEU:HD12	2.01	0.41
1:C:137:VAL:HG13	1:C:148:ILE:HG21	2.03	0.41
1:C:149:LYS:HE3	1:C:168:ARG:HD3	2.02	0.41
11:O:53:ARG:HA	11:O:56:LEU:HB3	2.03	0.41
5:A:1237:C:O2	5:A:1334:G:O2'	2.37	0.41
7:E:110:MET:HA	7:E:113:VAL:HG22	2.03	0.41
9:H:51:GLU:O	9:H:57:GLU:N	2.48	0.41
5:A:1254:A:O2'	5:A:1356:G:OP1	2.39	0.41
5:A:62:U:O2'	5:A:379:C:O2	2.29	0.41
5:A:451:A:H2	5:A:480:U:C2	2.38	0.41
5:A:829:G:H2'	5:A:830:G:H8	1.86	0.41
16:B:182:VAL:HB	16:B:195:VAL:HG13	2.03	0.41
1:C:63:ILE:HG23	1:C:96:VAL:HG11	2.03	0.41
9:H:83:ARG:HB2	13:Q:36:PHE:HE2	1.86	0.41
5:A:1000:A:N3	5:A:1041:G:N1	2.68	0.41
6:D:92:LEU:O	6:D:135:GLN:NE2	2.54	0.41
5:A:1072:G:H22	5:A:1104:G:H1'	1.85	0.41
5:A:81:A:N7	5:A:83:C:N4	2.69	0.41
5:A:908:A:H2'	5:A:909:A:C8	2.56	0.41
5:A:60:A:N7	5:A:108:G:O2'	2.54	0.41
15:T:28:ARG:HA	15:T:31:ILE:HD12	2.02	0.41
5:A:219:U:H2'	5:A:220:G:C8	2.55	0.40
1:C:145:ALA:O	1:C:147:GLY:N	2.54	0.40
14:R:62:ARG:HD2	14:R:69:TYR:HA	2.03	0.40
5:A:398:U:H2'	5:A:399:G:C8	2.56	0.40
7:E:81:GLN:HG2	7:E:82:HIS:HD2	1.86	0.40
8:F:11:HIS:CE1	8:F:13:ASP:HB2	2.56	0.40
5:A:878:A:P	9:H:79:ARG:HH11	2.44	0.40
1:C:13:ILE:HG22	1:C:14:VAL:H	1.85	0.40
2:J:11:LYS:HE3	2:J:71:LEU:HD21	2.03	0.40
12:P:28:ARG:HG2	12:P:29:ASN:H	1.85	0.40
5:A:1270:G:H2'	5:A:1271:A:C8	2.56	0.40
5:A:894:G:H1	5:A:905:U:H3	1.68	0.40
5:A:572:A:H5''	5:A:917:G:H4'	2.04	0.40
7:E:37:VAL:HA	7:E:47:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:11:LYS:HG2	2:J:71:LEU:HD23	2.02	0.40
5:A:331:G:O3'	15:T:2:ASN:HB3	2.21	0.40
15:T:53:MET:HA	15:T:56:ILE:HD12	2.03	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 PDB entries followed by that with respect to all EM entries.

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	C	204/206 (99%)	178 (87%)	26 (13%)	0	100	100
2	J	96/98 (98%)	76 (79%)	20 (21%)	0	100	100
3	N	92/99 (93%)	79 (86%)	13 (14%)	0	100	100
4	S	72/74 (97%)	67 (93%)	5 (7%)	0	100	100
6	D	203/205 (99%)	179 (88%)	24 (12%)	0	100	100
7	E	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
8	F	73/93 (78%)	68 (93%)	5 (7%)	0	100	100
9	H	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
10	L	121/123 (98%)	88 (73%)	33 (27%)	0	100	100
11	O	84/86 (98%)	75 (89%)	8 (10%)	1 (1%)	14	56
12	P	77/79 (98%)	61 (79%)	16 (21%)	0	100	100
13	Q	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
14	R	45/52 (86%)	45 (100%)	0	0	100	100
15	T	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
16	B	215/217 (99%)	181 (84%)	34 (16%)	0	100	100
All	All	1716/1774 (97%)	1481 (86%)	234 (14%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	46	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	C	170/170 (100%)	169 (99%)	1 (1%)	87	94
2	J	86/86 (100%)	86 (100%)	0	100	100
3	N	79/82 (96%)	77 (98%)	2 (2%)	50	77
4	S	65/65 (100%)	64 (98%)	1 (2%)	67	85
6	D	172/172 (100%)	169 (98%)	3 (2%)	63	84
7	E	111/112 (99%)	111 (100%)	0	100	100
8	F	69/82 (84%)	69 (100%)	0	100	100
9	H	104/104 (100%)	103 (99%)	1 (1%)	78	89
10	L	103/103 (100%)	103 (100%)	0	100	100
11	O	74/74 (100%)	73 (99%)	1 (1%)	69	86
12	P	64/64 (100%)	61 (95%)	3 (5%)	29	64
13	Q	73/73 (100%)	71 (97%)	2 (3%)	48	75
14	R	43/45 (96%)	43 (100%)	0	100	100
15	T	64/65 (98%)	64 (100%)	0	100	100
16	B	179/179 (100%)	178 (99%)	1 (1%)	87	94
All	All	1456/1476 (99%)	1441 (99%)	15 (1%)	80	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	184	ASN
3	N	27	LYS
3	N	60	ARG
4	S	28	LYS
6	D	151	GLN
6	D	176	LYS

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Mol	Chain	Res	Type
6	D	177	MET
9	H	93	LYS
11	O	53	ARG
12	P	5	ARG
12	P	28	ARG
12	P	51	ARG
13	Q	76	ARG
13	Q	80	LYS
16	B	224	ARG

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

Mol	Chain	Res	Type
1	C	24	ASN
15	T	74	HIS
16	B	119	GLN
16	B	121	GLN
16	B	202	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	1338/1542 (86%)	471 (35%)	15 (1%)

All (471) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	7	A
5	A	9	G
5	A	14	U
5	A	16	A
5	A	21	G
5	A	22	G
5	A	30	U
5	A	31	G
5	A	32	A
5	A	39	G
5	A	47	C
5	A	48	C
5	A	50	A

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Mol	Chain	Res	Type
5	A	51	A
5	A	52	C
5	A	58	C
5	A	60	A
5	A	61	G
5	A	66	A
5	A	69	G
5	A	70	U
5	A	71	A
5	A	72	A
5	A	75	G
5	A	76	G
5	A	83	C
5	A	84	U
5	A	85	U
5	A	86	G
5	A	87	C
5	A	88	U
5	A	89	U
5	A	95	C
5	A	108	G
5	A	110	C
5	A	112	G
5	A	119	A
5	A	120	A
5	A	121	U
5	A	125	U
5	A	130	A
5	A	131	A
5	A	134	G
5	A	135	C
5	A	136	C
5	A	144	G
5	A	145	G
5	A	151	A
5	A	163	C
5	A	173	U
5	A	174	A
5	A	175	C
5	A	177	G
5	A	182	A
5	A	196	A

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Mol	Chain	Res	Type
5	A	197	A
5	A	200	G
5	A	202	G
5	A	204	G
5	A	205	A
5	A	208	U
5	A	209	U
5	A	210	C
5	A	211	G
5	A	212	G
5	A	213	G
5	A	214	C
5	A	220	G
5	A	226	G
5	A	228	A
5	A	239	U
5	A	240	G
5	A	243	A
5	A	244	U
5	A	245	U
5	A	247	G
5	A	250	A
5	A	251	G
5	A	257	G
5	A	258	G
5	A	265	G
5	A	266	G
5	A	267	C
5	A	279	A
5	A	283	U
5	A	289	G
5	A	290	C
5	A	299	G
5	A	300	A
5	A	303	A
5	A	305	G
5	A	306	A
5	A	312	C
5	A	315	A
5	A	316	C
5	A	319	G
5	A	321	A

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Mol	Chain	Res	Type
5	A	328	C
5	A	329	A
5	A	332	G
5	A	336	A
5	A	337	G
5	A	339	C
5	A	345	C
5	A	347	G
5	A	348	G
5	A	350	G
5	A	351	G
5	A	352	C
5	A	353	A
5	A	354	G
5	A	362	G
5	A	367	U
5	A	368	U
5	A	369	G
5	A	372	C
5	A	373	A
5	A	375	U
5	A	380	G
5	A	381	C
5	A	382	A
5	A	397	A
5	A	398	U
5	A	406	G
5	A	407	U
5	A	408	A
5	A	411	A
5	A	412	A
5	A	413	G
5	A	414	A
5	A	415	A
5	A	417	G
5	A	421	U
5	A	422	C
5	A	423	G
5	A	424	G
5	A	429	U
5	A	435	A
5	A	439	U

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Mol	Chain	Res	Type
5	A	448	A
5	A	451	A
5	A	455	G
5	A	457	G
5	A	460	A
5	A	461	A
5	A	462	G
5	A	463	U
5	A	466	A
5	A	467	U
5	A	468	A
5	A	469	C
5	A	470	C
5	A	479	U
5	A	483	C
5	A	484	G
5	A	485	U
5	A	494	G
5	A	497	G
5	A	500	G
5	A	505	G
5	A	508	U
5	A	509	A
5	A	510	A
5	A	511	C
5	A	517	G
5	A	518	C
5	A	519	C
5	A	520	A
5	A	521	G
5	A	527	G
5	A	531	U
5	A	532	A
5	A	533	A
5	A	536	C
5	A	540	G
5	A	547	A
5	A	548	G
5	A	550	G
5	A	556	C
5	A	559	A
5	A	562	U

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Mol	Chain	Res	Type
5	A	564	C
5	A	567	G
5	A	572	A
5	A	573	A
5	A	576	C
5	A	577	G
5	A	580	C
5	A	581	G
5	A	582	C
5	A	587	G
5	A	588	G
5	A	602	A
5	A	604	G
5	A	606	G
5	A	607	A
5	A	610	U
5	A	620	C
5	A	623	C
5	A	633	G
5	A	641	U
5	A	642	A
5	A	646	G
5	A	652	U
5	A	653	U
5	A	654	G
5	A	661	G
5	A	663	A
5	A	665	A
5	A	666	G
5	A	667	G
5	A	671	G
5	A	673	A
5	A	674	G
5	A	675	A
5	A	677	U
5	A	678	U
5	A	713	G
5	A	714	G
5	A	717	U
5	A	718	A
5	A	721	G
5	A	722	G

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Mol	Chain	Res	Type
5	A	731	G
5	A	733	G
5	A	736	C
5	A	737	C
5	A	745	G
5	A	748	G
5	A	753	A
5	A	755	G
5	A	760	G
5	A	761	G
5	A	763	G
5	A	765	G
5	A	768	A
5	A	777	A
5	A	778	G
5	A	779	C
5	A	780	A
5	A	802	A
5	A	803	G
5	A	804	U
5	A	805	C
5	A	812	G
5	A	815	A
5	A	816	A
5	A	817	C
5	A	818	G
5	A	819	A
5	A	820	U
5	A	821	G
5	A	825	A
5	A	828	U
5	A	829	G
5	A	832	G
5	A	835	U
5	A	837	U
5	A	838	G
5	A	841	C
5	A	843	U
5	A	844	G
5	A	846	G
5	A	849	G
5	A	851	G

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Mol	Chain	Res	Type
5	A	853	C
5	A	857	C
5	A	858	G
5	A	865	A
5	A	867	G
5	A	873	A
5	A	876	C
5	A	885	G
5	A	890	G
5	A	895	G
5	A	900	A
5	A	901	A
5	A	914	A
5	A	918	A
5	A	921	U
5	A	922	G
5	A	926	G
5	A	927	G
5	A	930	C
5	A	931	C
5	A	934	C
5	A	942	G
5	A	945	G
5	A	948	C
5	A	953	G
5	A	954	G
5	A	955	U
5	A	958	A
5	A	960	U
5	A	961	U
5	A	962	C
5	A	963	G
5	A	966	G
5	A	968	A
5	A	969	A
5	A	971	G
5	A	972	C
5	A	973	G
5	A	974	A
5	A	975	A
5	A	976	G
5	A	977	A

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Mol	Chain	Res	Type
5	A	982	U
5	A	984	C
5	A	986	U
5	A	987	G
5	A	991	U
5	A	992	U
5	A	993	G
5	A	999	C
5	A	1004	A
5	A	1005	A
5	A	1010	U
5	A	1016	A
5	A	1020	G
5	A	1025	U
5	A	1026	G
5	A	1030	U
5	A	1032	G
5	A	1033	G
5	A	1034	G
5	A	1036	A
5	A	1037	C
5	A	1044	A
5	A	1045	C
5	A	1049	U
5	A	1052	U
5	A	1054	C
5	A	1055	A
5	A	1063	C
5	A	1064	G
5	A	1065	U
5	A	1066	C
5	A	1067	A
5	A	1070	U
5	A	1072	G
5	A	1077	G
5	A	1079	G
5	A	1080	A
5	A	1081	A
5	A	1085	U
5	A	1089	G
5	A	1091	U
5	A	1094	G

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Mol	Chain	Res	Type
5	A	1095	U
5	A	1098	C
5	A	1100	C
5	A	1101	A
5	A	1102	A
5	A	1105	A
5	A	1111	A
5	A	1112	C
5	A	1118	U
5	A	1119	C
5	A	1124	G
5	A	1125	U
5	A	1129	C
5	A	1133	G
5	A	1136	C
5	A	1137	C
5	A	1138	G
5	A	1139	G
5	A	1143	G
5	A	1145	A
5	A	1146	A
5	A	1152	A
5	A	1155	A
5	A	1157	A
5	A	1159	U
5	A	1160	G
5	A	1161	C
5	A	1168	U
5	A	1179	A
5	A	1181	G
5	A	1183	U
5	A	1184	G
5	A	1191	A
5	A	1193	G
5	A	1195	C
5	A	1197	A
5	A	1199	U
5	A	1200	C
5	A	1201	A
5	A	1202	U
5	A	1207	G
5	A	1209	C

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Mol	Chain	Res	Type
5	A	1210	C
5	A	1212	U
5	A	1213	A
5	A	1214	C
5	A	1215	G
5	A	1222	G
5	A	1224	U
5	A	1225	A
5	A	1226	C
5	A	1229	A
5	A	1230	C
5	A	1231	G
5	A	1236	A
5	A	1239	A
5	A	1240	U
5	A	1242	G
5	A	1243	C
5	A	1244	G
5	A	1246	A
5	A	1247	U
5	A	1248	A
5	A	1249	C
5	A	1253	G
5	A	1256	A
5	A	1257	A
5	A	1258	G
5	A	1260	G
5	A	1263	C
5	A	1265	C
5	A	1269	A
5	A	1270	G
5	A	1272	G
5	A	1274	A
5	A	1278	G
5	A	1280	A
5	A	1281	C
5	A	1285	A
5	A	1286	U
5	A	1290	G
5	A	1294	G
5	A	1296	C
5	A	1298	U

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Mol	Chain	Res	Type
5	A	1300	G
5	A	1301	U
5	A	1302	C
5	A	1304	G
5	A	1305	G
5	A	1309	G
5	A	1312	G
5	A	1313	U
5	A	1315	U
5	A	1316	G
5	A	1318	A
5	A	1319	A
5	A	1320	C
5	A	1322	C
5	A	1323	G
5	A	1324	A
5	A	1331	G
5	A	1332	A
5	A	1336	C
5	A	1337	G
5	A	1340	A
5	A	1347	G
5	A	1348	U
5	A	1350	A
5	A	1355	G
5	A	1362	A
5	A	1363	A
5	A	1364	U
5	A	1365	G
5	A	1368	A
5	A	1369	C
5	A	1378	C
5	A	1380	U
5	A	1381	U
5	A	1392	G
5	A	1394	A
5	A	1395	C
5	A	1396	A

All (15) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
5	A	51	A
5	A	238	A
5	A	243	A
5	A	328	C
5	A	372	C
5	A	428	G
5	A	484	G
5	A	913	A
5	A	929	G
5	A	930	C
5	A	1065	U
5	A	1101	A
5	A	1201	A
5	A	1213	A
5	A	1300	G

## 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.