



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 01:13 PM UTC

PDB ID : 7ACS / pdb_00007acs
BMRB ID : 34511
Title : The SARS-CoV-2 nucleocapsid phosphoprotein N-terminal domain in complex with 7mer dsRNA
Authors : Veverka, V.
Deposited on : 2020-09-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

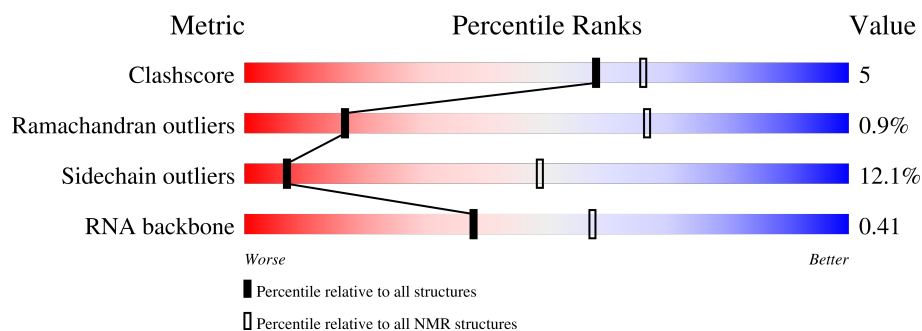
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823
RNA backbone	8273	777

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	A	140	
2	B	7	
3	C	7	

2 Ensemble composition and analysis

This entry contains 30 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:10-A:55, A:61-A:136 (122)	0.56	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 11 single-model clusters were found.

Cluster number	Models
1	3, 4, 8, 9, 10, 11, 13, 14, 18, 20, 22, 23, 24, 25, 27
2	6, 30
3	7, 26
Single-model clusters	1; 2; 5; 12; 15; 16; 17; 19; 21; 28; 29

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2564 atoms, of which 1195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2109	671	1040	195	201	2	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0DTC9
A	2	ALA	-	expression tag	UNP P0DTC9
A	3	MET	-	expression tag	UNP P0DTC9

- Molecule 2 is a RNA chain called RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	7	Total	C	H	N	O	P	0
			226	66	78	26	49	7	

- Molecule 3 is a RNA chain called RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3').

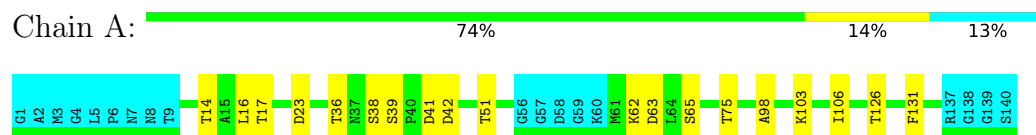
Mol	Chain	Residues	Atoms						Trace
3	C	7	Total	C	H	N	O	P	0
			229	67	77	27	51	7	

4 Residue-property plots [i](#)

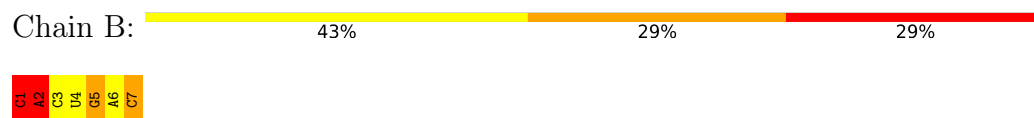
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

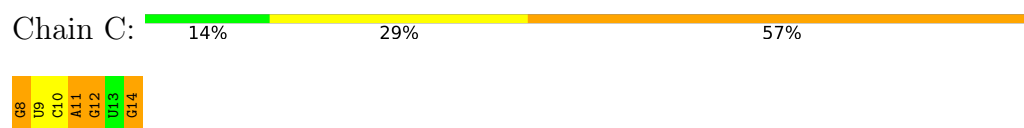
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')



- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

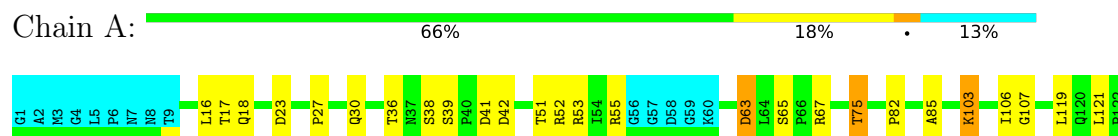


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Nucleoprotein





- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

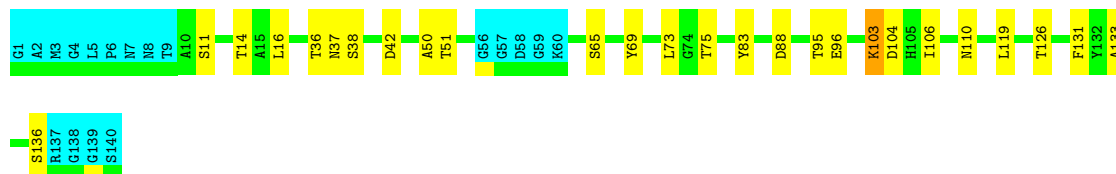


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

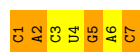


4.2.2 Score per residue for model 2

- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')



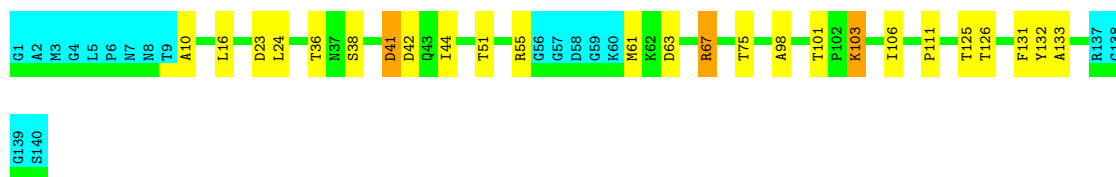
- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.3 Score per residue for model 3

- Molecule 1: Nucleoprotein





- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')



- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

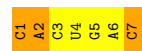


4.2.4 Score per residue for model 4

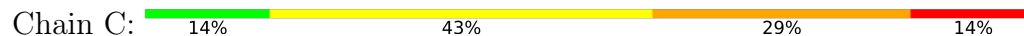
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

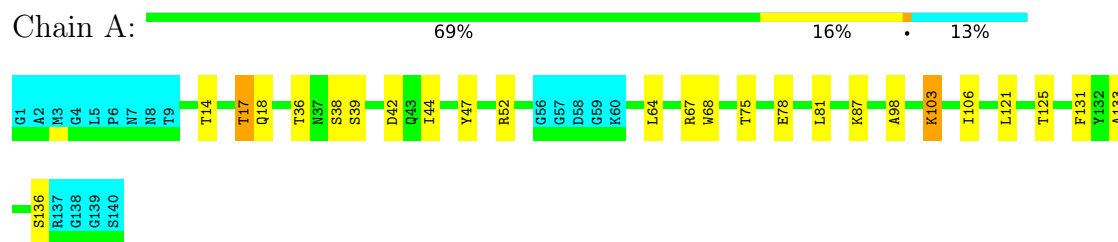


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

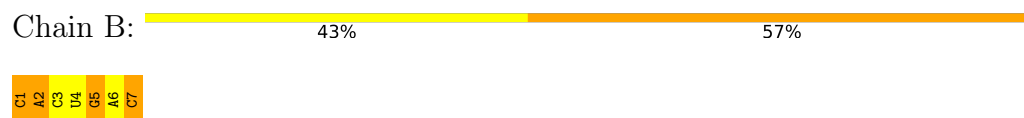


4.2.5 Score per residue for model 5

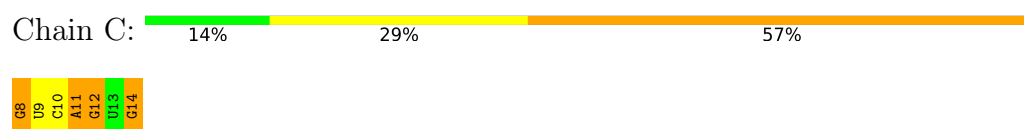
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

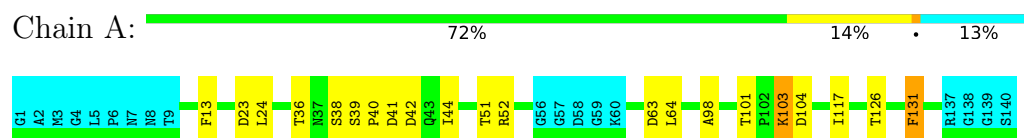


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

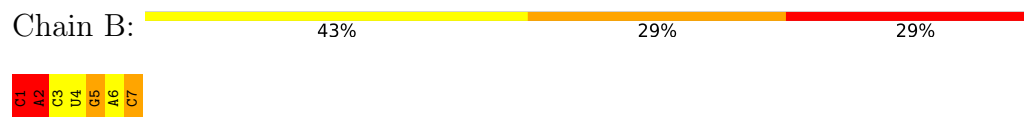


4.2.6 Score per residue for model 6

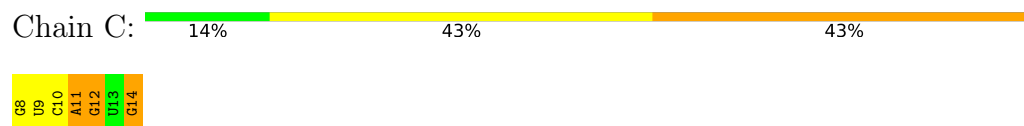
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

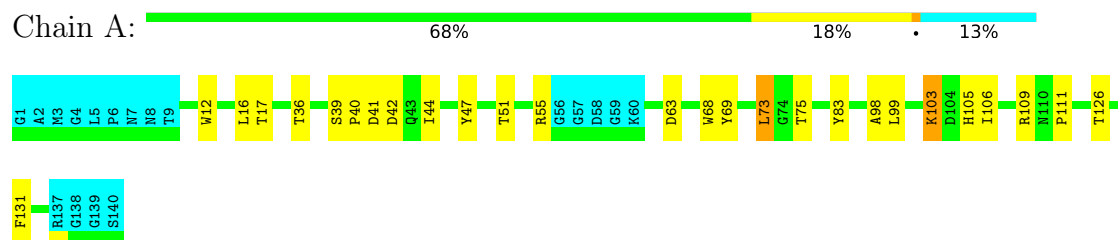


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

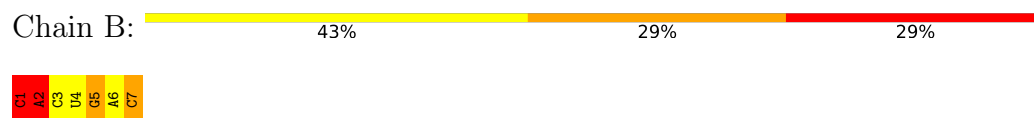


4.2.7 Score per residue for model 7

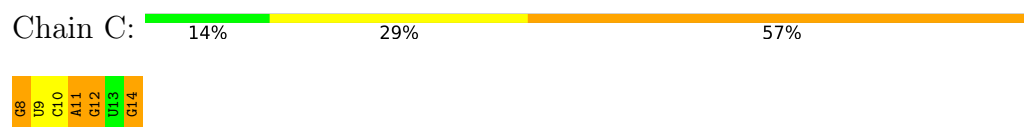
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

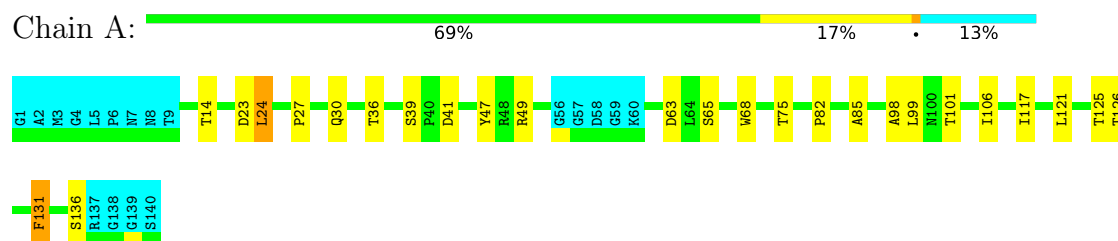


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

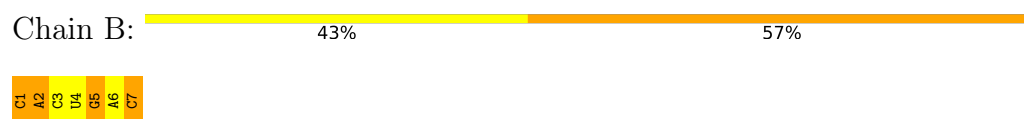


4.2.8 Score per residue for model 8

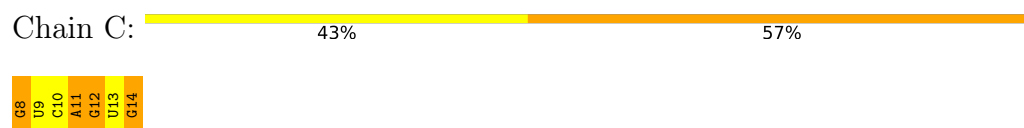
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

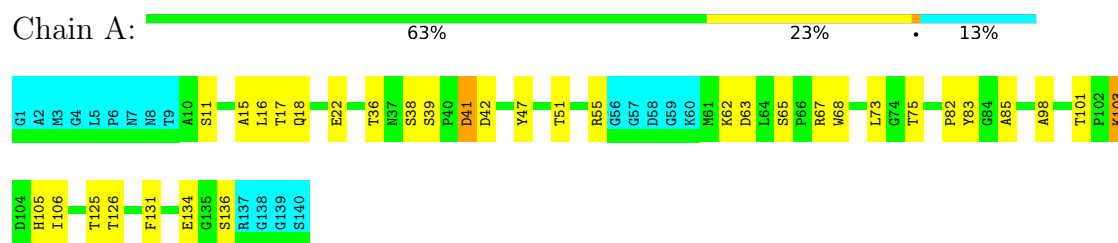


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

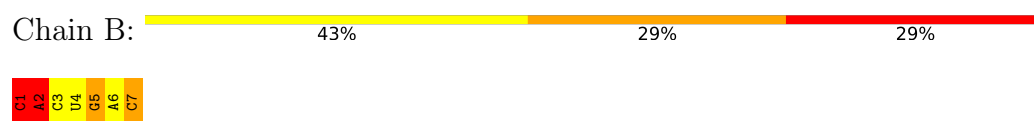


4.2.9 Score per residue for model 9

- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

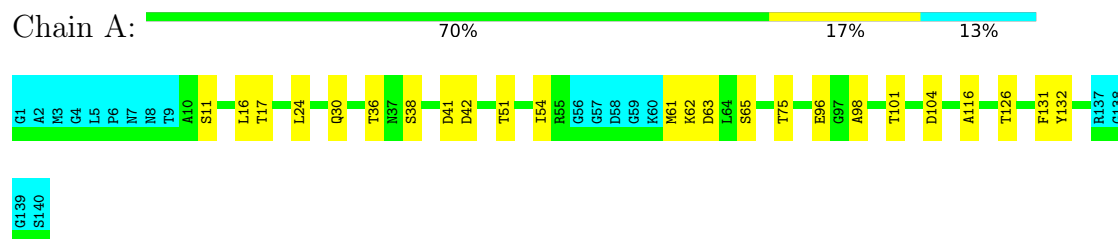


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

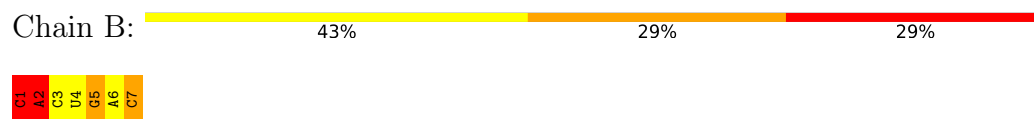


4.2.10 Score per residue for model 10

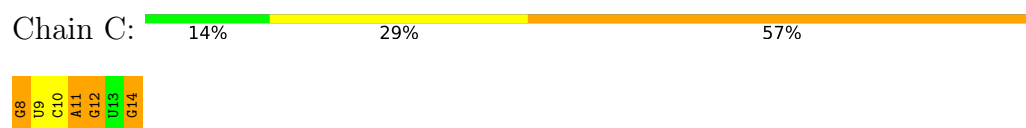
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')



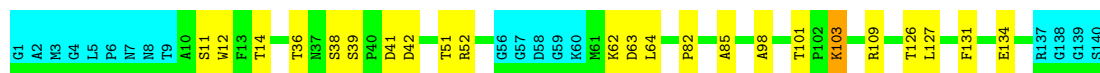
- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.11 Score per residue for model 11

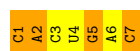
- Molecule 1: Nucleoprotein

Chain A: 71% 16% 13%



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

Chain B: 43% 57%



- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

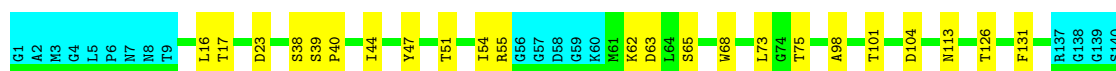
Chain C: 14% 43% 43%



4.2.12 Score per residue for model 12

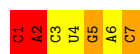
- Molecule 1: Nucleoprotein

Chain A: 71% 16% 13%



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

Chain B: 43% 29% 29%



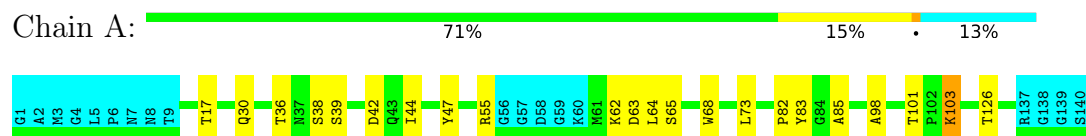
- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

Chain C: 14% 43% 43%



4.2.13 Score per residue for model 13 (medoid)

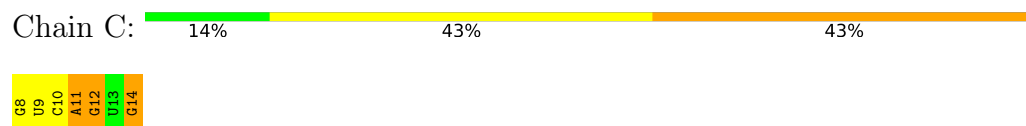
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

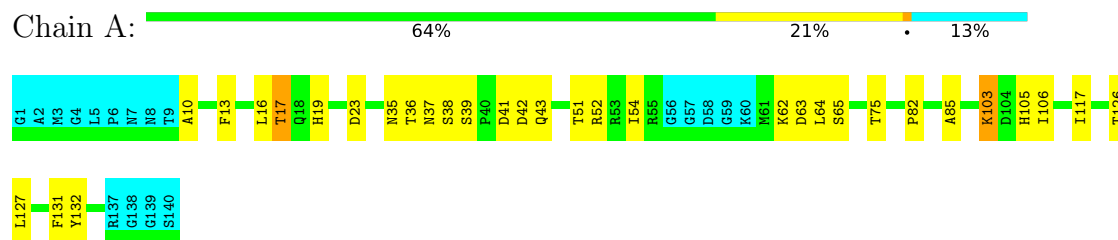


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.14 Score per residue for model 14

- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

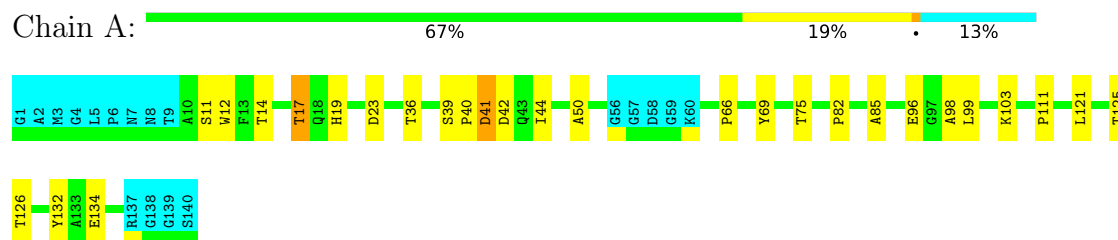


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

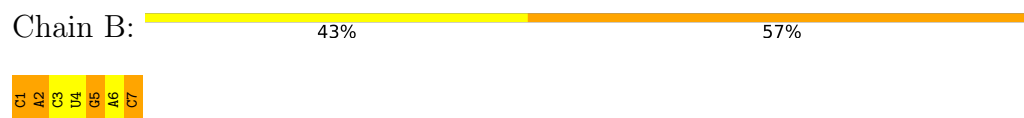


4.2.15 Score per residue for model 15

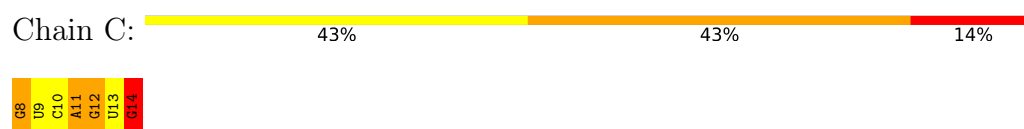
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

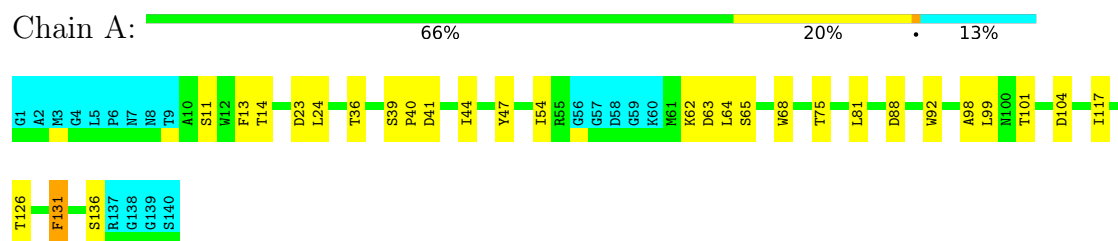


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

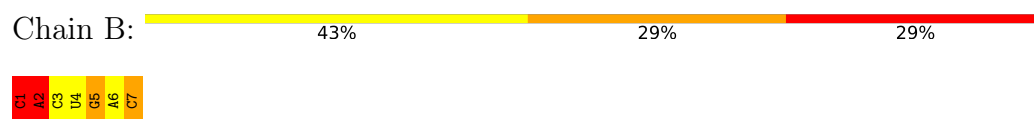


4.2.16 Score per residue for model 16

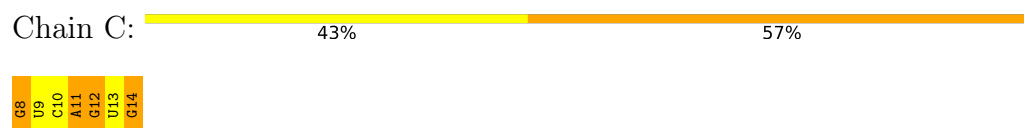
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

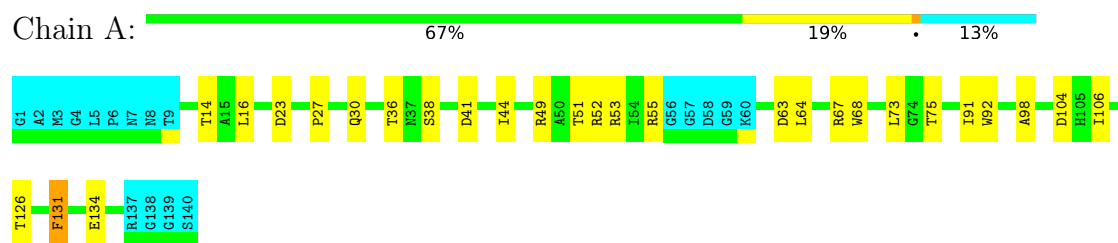


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

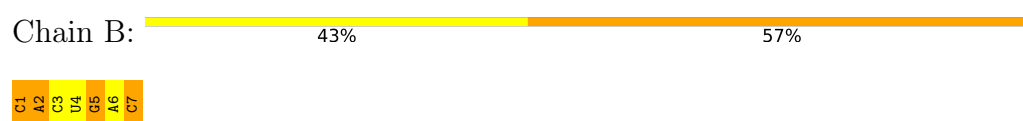


4.2.17 Score per residue for model 17

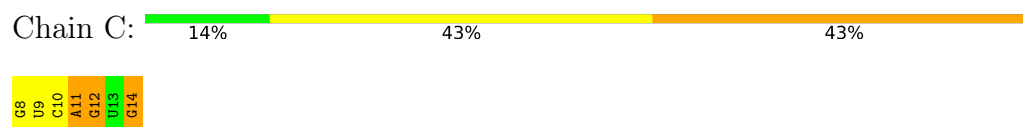
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

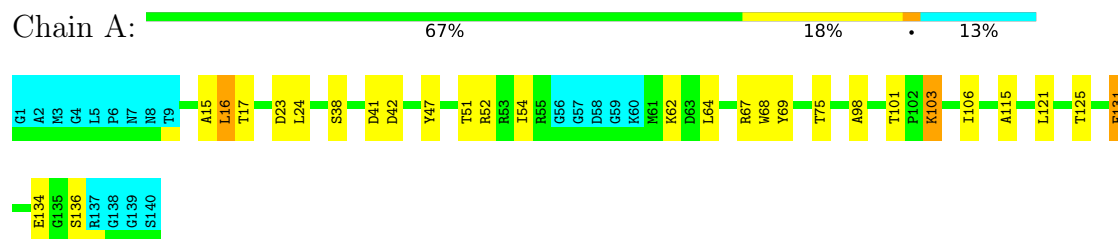


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

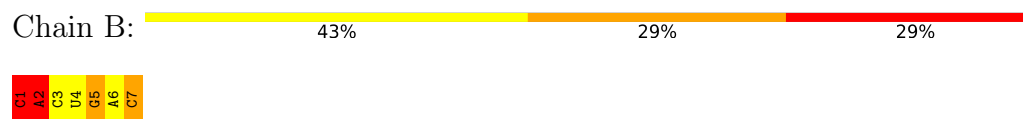


4.2.18 Score per residue for model 18

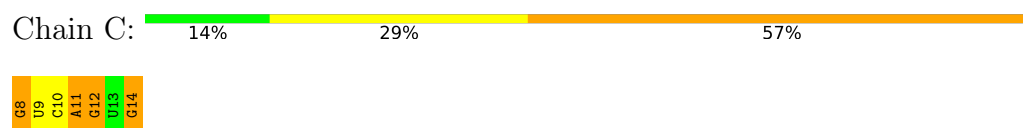
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

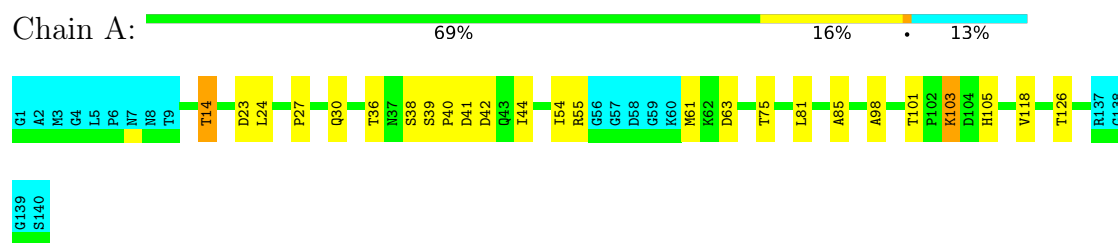


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.19 Score per residue for model 19

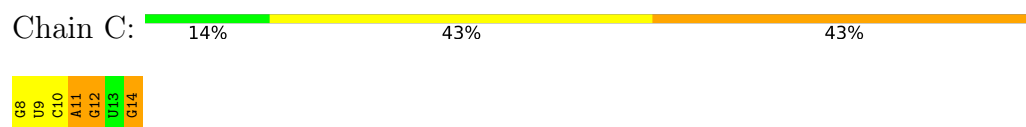
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

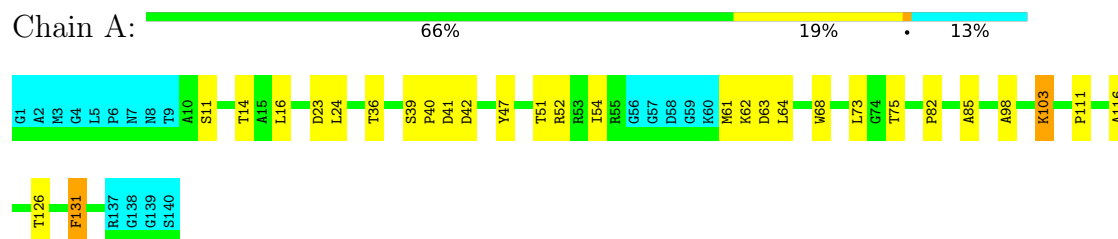


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

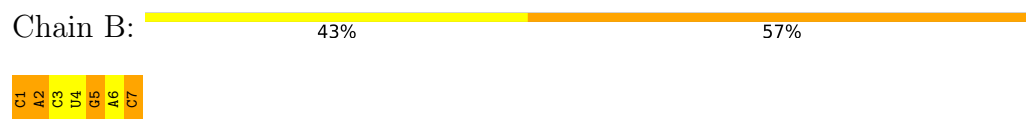


4.2.20 Score per residue for model 20

- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

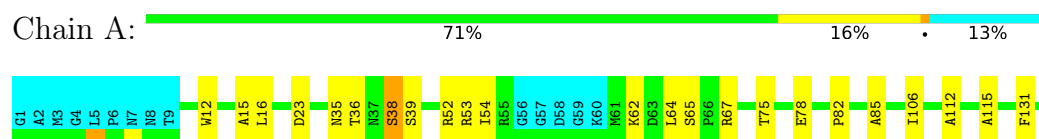


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.21 Score per residue for model 21

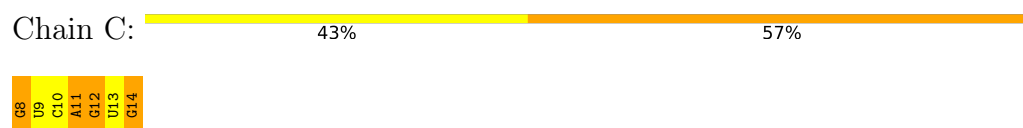
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

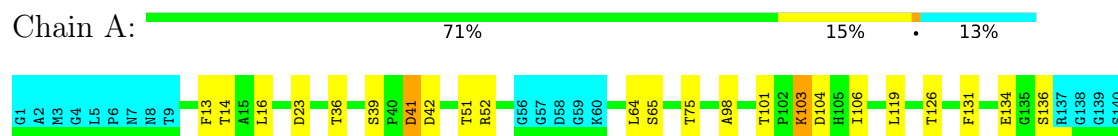


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

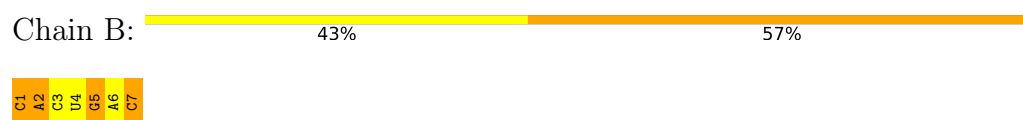


4.2.22 Score per residue for model 22

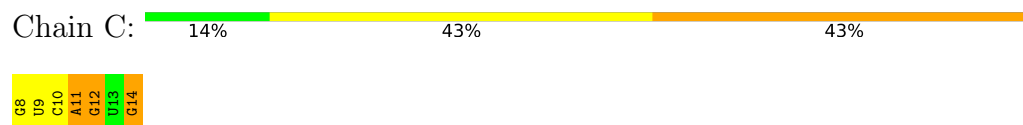
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

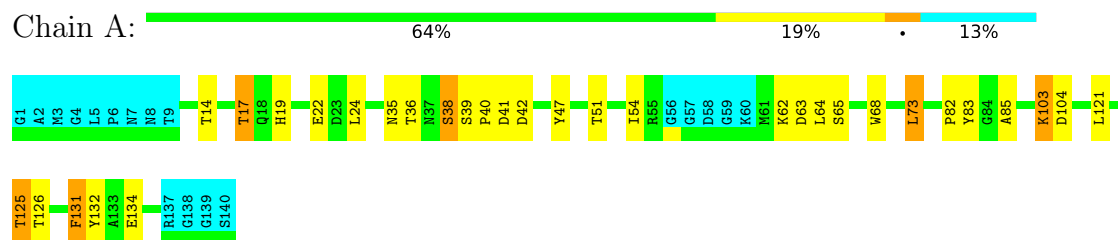


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.23 Score per residue for model 23

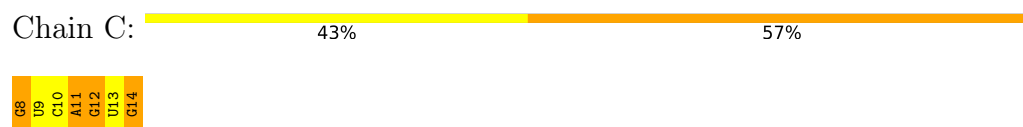
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

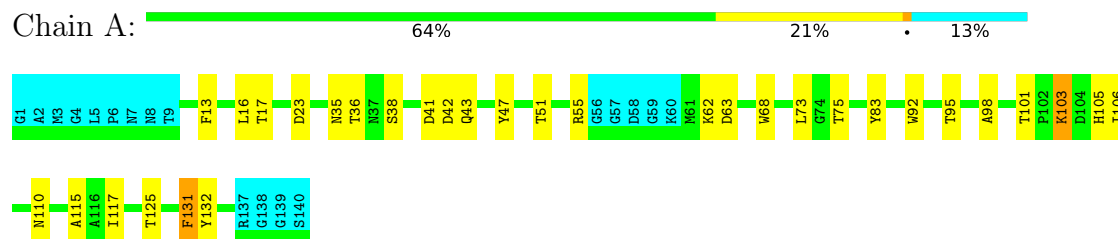


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.24 Score per residue for model 24

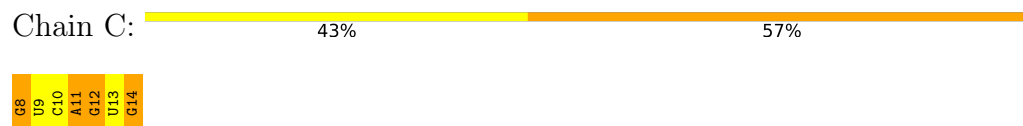
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

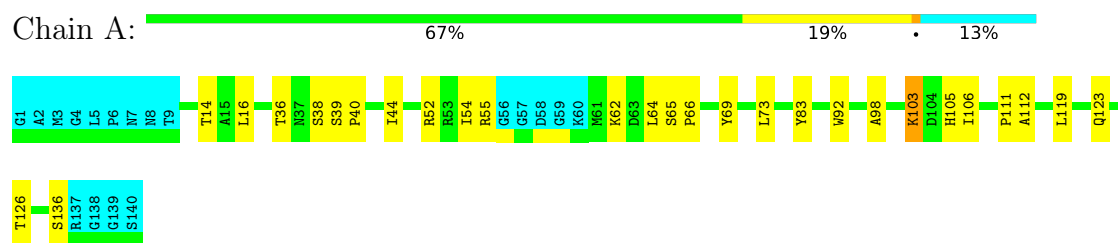


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

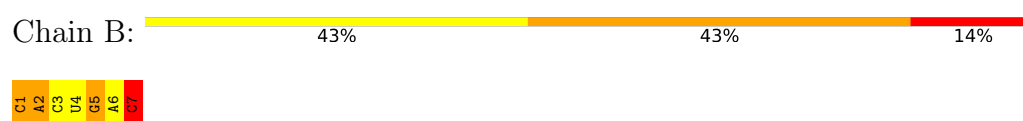


4.2.25 Score per residue for model 25

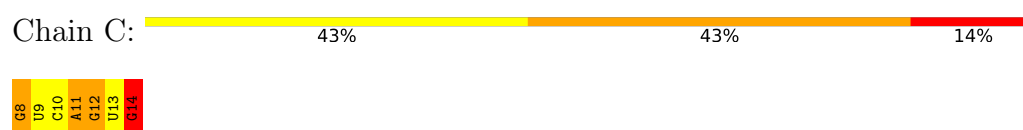
• Molecule 1: Nucleoprotein



• Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

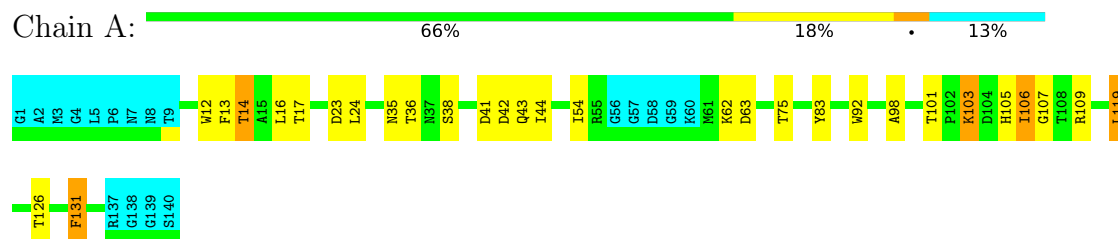


• Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

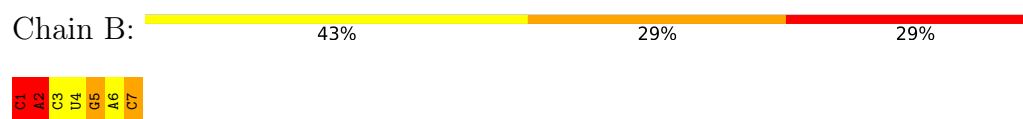


4.2.26 Score per residue for model 26

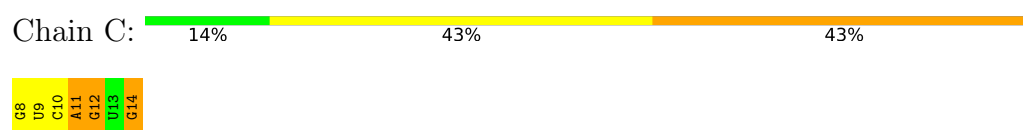
• Molecule 1: Nucleoprotein



• Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

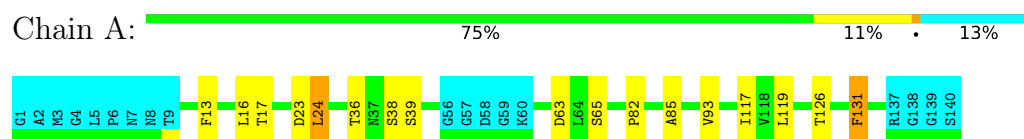


• Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.27 Score per residue for model 27

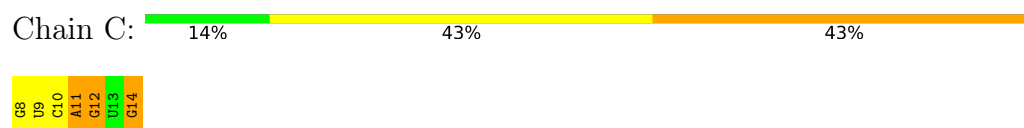
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

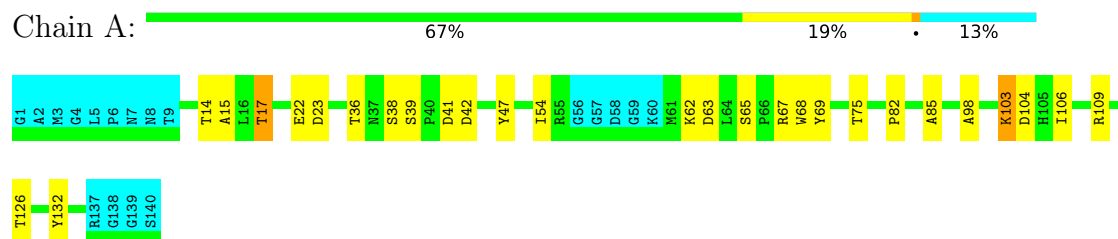


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.28 Score per residue for model 28

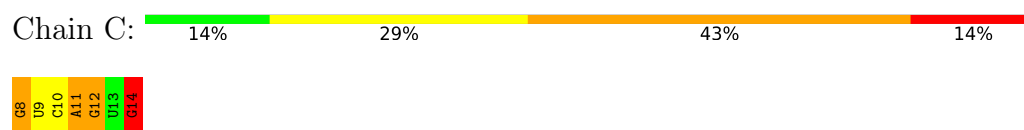
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

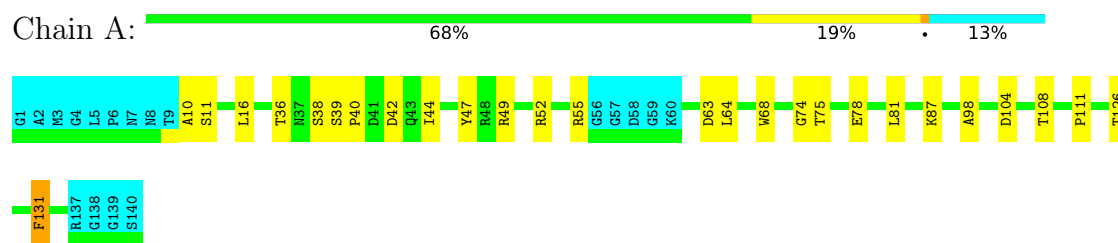


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')

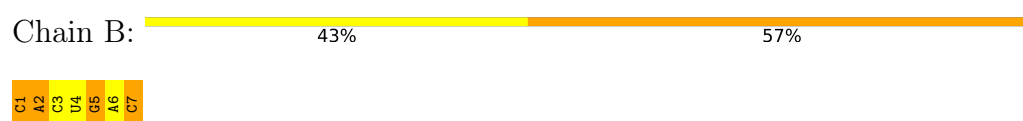


4.2.29 Score per residue for model 29

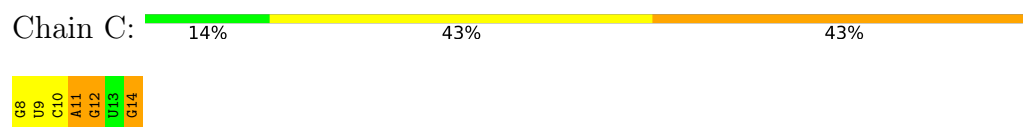
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')

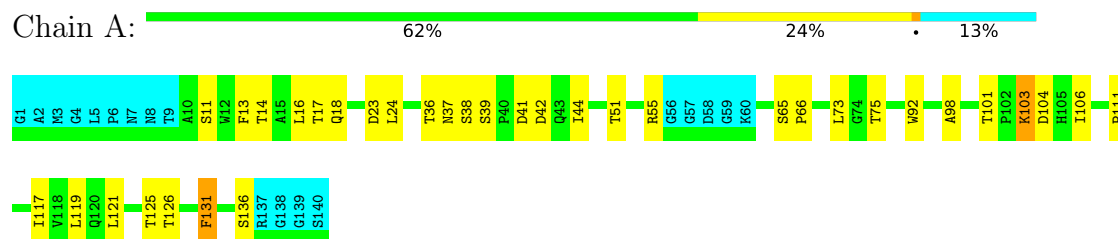


- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



4.2.30 Score per residue for model 30

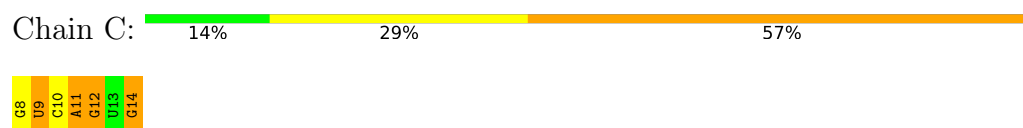
- Molecule 1: Nucleoprotein



- Molecule 2: RNA (5'-R(P*CP*AP*CP*UP*GP*AP*C)-3')



- Molecule 3: RNA (5'-R(P*GP*UP*CP*AP*GP*UP*G)-3')



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality i

6.1 Standard geometry i

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 (average) 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	0.33±0.01	0±0/984 (0.0± 0.0%)	0.67±0.02	0±0/1341 (0.0± 0.0%)
2	B	1.83±0.00	2±0/164 (1.2± 0.0%)	2.03±0.00	8±0/251 (3.1± 0.2%)
3	C	1.78±0.00	1±0/169 (0.6± 0.0%)	2.07±0.00	8±0/260 (3.2± 0.2%)
All	All	0.95	90/39510 (0.2%)	1.22	482/55560 (0.9%)

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	Planarity
2	B	0.0±0.0	3.0±0.0
3	C	0.0±0.0	4.0±0.0
All	All	0	210

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	8	G	OP3-P	5.69	1.59	1.48	24	30
2	B	1	C	OP3-P	5.66	1.59	1.48	17	30
2	B	7	C	C3'-O3'	5.47	1.50	1.42	6	30

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	8	G	O4'-C4'-C3'	11.05	115.05	104.00	3	30
3	C	12	G	C4'-C3'-C2'	-8.34	94.26	102.60	3	30
3	C	9	U	O3'-P-O5'	8.28	116.42	104.00	21	30
2	B	6	A	O4'-C4'-C3'	7.57	111.57	104.00	20	30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	11	A	C1'-C2'-O2'	6.83	118.64	108.40	30	30
3	C	9	U	O4'-C1'-N1	6.80	118.71	108.50	25	30
3	C	8	G	C4'-C3'-C2'	-6.64	95.96	102.60	22	30
3	C	14	G	O4'-C4'-C3'	5.73	109.73	104.00	9	30
2	B	3	C	N1-C1'-C2'	-5.72	103.42	112.00	1	30
2	B	2	A	N9-C1'-C2'	-5.70	103.44	112.00	3	30
2	B	1	C	C4'-C3'-C2'	-5.63	96.97	102.60	27	30
2	B	4	U	O4'-C1'-N1	5.50	116.76	108.50	5	30
2	B	4	U	O4'-C4'-C3'	5.40	109.40	104.00	24	30
2	B	6	A	C3'-C2'-O2'	5.27	118.61	110.70	15	30
3	C	12	G	O3'-P-O5'	5.22	111.83	104.00	9	30
2	B	5	G	C4'-C3'-C2'	-5.09	97.51	102.60	17	24
3	C	9	U	O4'-C4'-C3'	5.05	109.05	104.00	26	8

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	2	A	Sidechain	30
2	B	5	G	Sidechain	30
2	B	7	C	Sidechain	30
3	C	10	C	Sidechain	30
3	C	11	A	Sidechain	30
3	C	12	G	Sidechain	30
3	C	14	G	Sidechain	30

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	955	931	929	10±3
2	B	148	78	73	1±1
3	C	152	77	72	1±1
All	All	37650	32580	32220	325

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 5.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:HG22	3:C:8:G:H5'	0.84	1.48	23	4
1:A:42:ASP:HA	1:A:103:LYS:HE3	0.81	1.52	11	20
1:A:14:THR:HB	1:A:134:GLU:HB3	0.75	1.59	15	4
1:A:44:ILE:HB	1:A:98:ALA:HB1	0.72	1.61	19	14
1:A:54:ILE:HG12	1:A:62:LYS:HB2	0.71	1.61	12	6
1:A:41:ASP:HA	1:A:98:ALA:HA	0.67	1.65	4	11
1:A:132:TYR:HE1	2:B:1:C:H5'	0.66	1.50	3	1
1:A:111:PRO:HB2	3:C:9:U:H5'	0.64	1.69	20	2
1:A:16:LEU:HB3	1:A:131:PHE:HE2	0.64	1.53	27	4
1:A:16:LEU:HB3	1:A:131:PHE:CE2	0.63	2.28	27	10
1:A:16:LEU:HB3	1:A:131:PHE:HZ	0.63	1.54	12	1
1:A:16:LEU:HD11	1:A:119:LEU:HD13	0.62	1.70	25	1
1:A:52:ARG:HB3	1:A:64:LEU:HD12	0.61	1.72	20	11
1:A:13:PHE:HD1	1:A:119:LEU:HA	0.60	1.54	22	2
1:A:18:GLN:HB3	1:A:66:PRO:HB2	0.60	1.74	30	1
1:A:16:LEU:HB3	1:A:131:PHE:CZ	0.59	2.31	12	3
1:A:62:LYS:HA	3:C:14:G:O6	0.59	1.98	28	2
1:A:27:PRO:HG2	1:A:30:GLN:HB3	0.59	1.73	8	3
1:A:39:SER:HB3	1:A:40:PRO:HD2	0.59	1.74	23	10
1:A:101:THR:O	1:A:103:LYS:HD2	0.58	1.99	24	10
1:A:10:ALA:HB2	1:A:111:PRO:HB3	0.58	1.75	29	1
1:A:103:LYS:HB2	1:A:105:HIS:HD2	0.56	1.61	7	2
1:A:24:LEU:HD13	1:A:131:PHE:CE1	0.55	2.36	30	8
1:A:73:LEU:HD11	1:A:83:TYR:HB2	0.55	1.76	23	7
1:A:47:TYR:HB3	1:A:68:TRP:CE3	0.55	2.37	5	8
1:A:132:TYR:CE1	2:B:1:C:H5'	0.55	2.35	3	1
1:A:17:THR:HB	1:A:132:TYR:CE1	0.55	2.37	15	3
1:A:19:HIS:HB2	1:A:132:TYR:HE2	0.54	1.63	23	2
1:A:17:THR:HG23	1:A:67:ARG:HG2	0.54	1.79	5	1
1:A:82:PRO:HD2	1:A:85:ALA:HB2	0.54	1.77	23	13
1:A:47:TYR:HB3	1:A:68:TRP:HE3	0.54	1.62	23	14
1:A:81:LEU:HB3	1:A:92:TRP:HH2	0.53	1.61	16	1
1:A:41:ASP:HB2	1:A:99:LEU:HG	0.52	1.79	7	4
1:A:62:LYS:HG3	2:B:1:C:N4	0.52	2.19	23	1
1:A:17:THR:HB	1:A:132:TYR:CE2	0.52	2.40	10	2
1:A:16:LEU:HD21	1:A:119:LEU:HD22	0.52	1.82	1	2
1:A:50:ALA:HB3	1:A:69:TYR:HE2	0.51	1.65	2	1
1:A:50:ALA:HB3	1:A:69:TYR:CE2	0.50	2.41	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ILE:HG12	1:A:62:LYS:H	0.49	1.67	25	2
1:A:24:LEU:HD13	1:A:131:PHE:HE1	0.49	1.68	30	1
1:A:75:THR:HG22	1:A:107:GLY:HA3	0.49	1.85	26	2
1:A:69:TYR:HE1	3:C:8:G:H5''	0.49	1.66	15	4
1:A:13:PHE:HA	1:A:117:ILE:O	0.49	2.08	27	5
1:A:87:LYS:HD2	1:A:90:ILE:HG13	0.49	1.84	4	1
1:A:27:PRO:HG2	1:A:30:GLN:HB2	0.49	1.85	4	2
1:A:133:ALA:HB3	1:A:136:SER:HB2	0.49	1.84	2	1
1:A:95:THR:HG22	1:A:98:ALA:HB2	0.49	1.85	24	1
1:A:15:ALA:HB1	1:A:67:ARG:HB2	0.48	1.85	21	2
1:A:55:ARG:HA	1:A:55:ARG:HE	0.48	1.68	24	1
1:A:115:ALA:HA	3:C:8:G:H1'	0.48	1.85	24	3
1:A:111:PRO:HB2	3:C:9:U:C5'	0.47	2.39	20	1
1:A:42:ASP:HA	1:A:103:LYS:CE	0.47	2.39	1	2
1:A:73:LEU:HG	1:A:92:TRP:HZ3	0.47	1.69	30	4
1:A:112:ALA:HA	3:C:8:G:N2	0.47	2.24	21	1
1:A:121:LEU:HB3	1:A:125:THR:HB	0.47	1.86	8	4
1:A:15:ALA:HB1	1:A:67:ARG:HB3	0.47	1.87	28	2
1:A:14:THR:OG1	1:A:118:VAL:HA	0.47	2.10	19	1
1:A:103:LYS:HG3	1:A:106:ILE:HD11	0.47	1.86	26	1
1:A:18:GLN:HB2	1:A:131:PHE:CE1	0.47	2.43	9	1
1:A:35:ASN:HB3	1:A:38:SER:OG	0.47	2.10	21	2
1:A:81:LEU:HD21	1:A:87:LYS:HD2	0.46	1.87	5	2
1:A:19:HIS:HB2	1:A:132:TYR:CE2	0.46	2.45	23	2
1:A:10:ALA:HB1	3:C:8:G:O2'	0.46	2.11	3	2
1:A:121:LEU:HD13	1:A:125:THR:HG22	0.46	1.88	30	3
1:A:18:GLN:HB2	1:A:131:PHE:CZ	0.46	2.46	1	2
1:A:116:ALA:HB3	3:C:8:G:H4'	0.46	1.87	20	2
1:A:16:LEU:HD23	1:A:133:ALA:HB2	0.46	1.87	3	1
1:A:73:LEU:HG	1:A:92:TRP:CZ3	0.45	2.46	30	4
1:A:12:TRP:HA	1:A:109:ARG:HD3	0.45	1.87	26	1
1:A:111:PRO:HB2	3:C:8:G:N3	0.45	2.27	3	4
1:A:103:LYS:HB2	1:A:105:HIS:CD2	0.45	2.47	14	5
1:A:127:LEU:HD22	1:A:131:PHE:HD2	0.44	1.72	11	1
1:A:16:LEU:HB2	1:A:131:PHE:CZ	0.44	2.48	10	1
1:A:12:TRP:CD2	1:A:109:ARG:HD3	0.44	2.48	7	1
1:A:83:TYR:CE1	1:A:92:TRP:HB3	0.44	2.48	26	1
1:A:54:ILE:HD11	3:C:13:U:H5	0.43	1.73	23	1
1:A:69:TYR:OH	3:C:8:G:H5''	0.43	2.12	18	1
1:A:14:THR:HB	1:A:134:GLU:HB2	0.43	1.89	23	1
1:A:35:ASN:HB2	1:A:43:GLN:OE1	0.43	2.14	24	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ALA:HB1	2:B:7:C:H2'	0.43	1.90	25	1
1:A:17:THR:HB	1:A:132:TYR:CZ	0.43	2.48	28	1
1:A:13:PHE:CD1	1:A:119:LEU:HA	0.43	2.42	22	1
1:A:112:ALA:HA	3:C:8:G:H21	0.43	1.74	21	1
1:A:134:GLU:OE1	1:A:134:GLU:HA	0.42	2.13	4	1
1:A:13:PHE:CD1	1:A:117:ILE:HB	0.42	2.49	30	1
1:A:53:ARG:HG3	1:A:63:ASP:HA	0.42	1.91	1	2
1:A:62:LYS:HE3	1:A:64:LEU:HD21	0.42	1.90	20	3
1:A:62:LYS:HG3	3:C:13:U:O4	0.42	2.15	20	3
1:A:24:LEU:HB2	1:A:131:PHE:CZ	0.42	2.49	6	1
1:A:67:ARG:HH21	1:A:134:GLU:CD	0.42	2.22	17	1
1:A:62:LYS:HE3	3:C:13:U:O4	0.42	2.15	9	1
1:A:134:GLU:HG2	3:C:8:G:OP1	0.41	2.14	18	1
1:A:69:TYR:CE1	3:C:8:G:H5''	0.41	2.49	15	1
1:A:133:ALA:HB3	1:A:136:SER:HB3	0.41	1.92	5	1
1:A:69:TYR:HE1	3:C:8:G:C5'	0.41	2.26	7	1
1:A:68:TRP:CZ3	1:A:91:ILE:HG12	0.41	2.51	17	1
1:A:74:GLY:O	1:A:104:ASP:HB3	0.41	2.15	29	1
1:A:16:LEU:HG	1:A:119:LEU:HD13	0.41	1.91	27	1
1:A:81:LEU:HB3	1:A:92:TRP:CH2	0.41	2.47	16	1
1:A:54:ILE:O	1:A:61:MET:HG2	0.41	2.16	20	1
2:B:1:C:N4	2:B:2:A:N6	0.41	2.70	23	17
1:A:16:LEU:O	1:A:67:ARG:HA	0.41	2.16	3	1
1:A:81:LEU:HG	1:A:85:ALA:HB3	0.40	1.93	19	1
1:A:23:ASP:O	1:A:24:LEU:HB2	0.40	2.16	27	1
1:A:12:TRP:CE2	1:A:109:ARG:HD3	0.40	2.51	11	1
1:A:16:LEU:HD13	1:A:131:PHE:HE2	0.40	1.76	22	1
1:A:43:GLN:HB2	1:A:95:THR:HG21	0.40	1.93	24	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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 NMR 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	A	122/140 (87%)	111±3 (91±2%)	10±3 (8±2%)	1±1 (1±1%)	16	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3660/4200 (87%)	3322 (91%)	304 (8%)	34 (1%)	16	66

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	63	ASP	21
1	A	24	LEU	5
1	A	37	ASN	3
1	A	66	PRO	2
1	A	113	ASN	1
1	A	123	GLN	1
1	A	14	THR	1

6.3.2 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 NMR 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	A	97/107 (91%)	85±3 (88±3%)	12±3 (12±3%)	7	49
All	All	2910/3210 (91%)	2558 (88%)	352 (12%)	7	49

All 46 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	THR	28
1	A	126	THR	25
1	A	38	SER	24
1	A	75	THR	23
1	A	103	LYS	20
1	A	23	ASP	18
1	A	51	THR	18
1	A	106	ILE	18
1	A	65	SER	17
1	A	17	THR	14
1	A	41	ASP	14
1	A	131	PHE	14

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Mol	Chain	Res	Type	Models (Total)
1	A	39	SER	13
1	A	55	ARG	11
1	A	104	ASP	10
1	A	11	SER	9
1	A	14	THR	7
1	A	136	SER	7
1	A	125	THR	6
1	A	73	LEU	5
1	A	101	THR	5
1	A	96	GLU	3
1	A	61	MET	3
1	A	12	TRP	3
1	A	78	GLU	3
1	A	49	ARG	3
1	A	22	GLU	3
1	A	54	ILE	3
1	A	67	ARG	2
1	A	88	ASP	2
1	A	110	ASN	2
1	A	119	LEU	2
1	A	30	GLN	2
1	A	42	ASP	2
1	A	64	LEU	2
1	A	52	ARG	1
1	A	123	GLN	1
1	A	95	THR	1
1	A	117	ILE	1
1	A	134	GLU	1
1	A	127	LEU	1
1	A	19	HIS	1
1	A	16	LEU	1
1	A	53	ARG	1
1	A	93	VAL	1
1	A	109	ARG	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	7/7 (100%)	0±0 (0±0%)	1±0 (14±0%)	0.48±0.00
3	C	6/7 (86%)	0±0 (0±0%)	0±0 (0±0%)	0.35±0.00
All	All	390/420 (93%)	0 (0%)	30 (8%)	0.41

The overall RNA backbone suiteness is 0.41.

There are no RNA backbone outliers to report.

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	1	C	30

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	24

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	0.17 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.03 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.10 ± 0.15	None needed (< 0.5 ppm)
^{15}N	127	-0.56 ± 0.42	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1495 atoms were assigned a chemical shift out of a possible 1901. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	600/604 (99%)	247/248 (100%)	242/244 (99%)	111/112 (99%)
Sidechain	791/878 (90%)	535/569 (94%)	236/267 (88%)	20/42 (48%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	104/155 (67%)	63/74 (85%)	38/74 (51%)	3/7 (43%)
Sugar	0/154 (0%)	0/84 (0%)	0/70 (0%)	0/0 (—%)
Base	0/110 (0%)	0/68 (0%)	0/24 (0%)	0/18 (0%)
Overall	1495/1901 (79%)	845/1043 (81%)	516/679 (76%)	134/179 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1660 atoms were assigned a chemical shift out of a possible 2090. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	691/699 (99%)	287/290 (99%)	277/280 (99%)	127/129 (98%)
Sidechain	865/972 (89%)	585/629 (93%)	259/295 (88%)	21/48 (44%)
Aromatic	104/155 (67%)	63/74 (85%)	38/74 (51%)	3/7 (43%)
Sugar	0/154 (0%)	0/84 (0%)	0/70 (0%)	0/0 (—%)
Base	0/110 (0%)	0/68 (0%)	0/24 (0%)	0/18 (0%)
Overall	1660/2090 (79%)	935/1145 (82%)	574/743 (77%)	151/202 (75%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	72	TYR	CE1	182.76	111.24 – 124.66	48.3
1	A	14	THR	HG1	6.34	0.08 – 2.19	24.6
1	A	125	THR	HG1	5.79	0.08 – 2.19	22.1
1	A	101	THR	HG1	5.78	0.08 – 2.19	22.0
1	A	47	TYR	CE1	129.73	111.24 – 124.66	8.8
1	A	109	ARG	HB3	-0.55	0.43 – 3.11	-8.6
1	A	49	ARG	HB3	-0.51	0.43 – 3.11	-8.5
1	A	47	TYR	HE1	5.00	5.59 – 7.82	-7.6
1	A	47	TYR	HE2	5.00	5.58 – 7.83	-7.5
1	A	24	LEU	HD11	-1.21	-0.61 – 2.12	-7.2
1	A	24	LEU	HD12	-1.21	-0.61 – 2.12	-7.2
1	A	24	LEU	HD13	-1.21	-0.61 – 2.12	-7.2
1	A	33	PRO	HD3	0.96	1.76 – 5.48	-7.1
1	A	24	LEU	HB3	-0.85	-0.26 – 3.31	-6.7
1	A	78	GLU	HB2	0.69	1.00 – 3.05	-6.5
1	A	33	PRO	HG3	-0.10	0.33 – 3.48	-6.3
1	A	31	GLY	HA2	1.75	2.15 – 5.77	-6.1
1	A	24	LEU	HB2	-0.33	-0.07 – 3.30	-5.8

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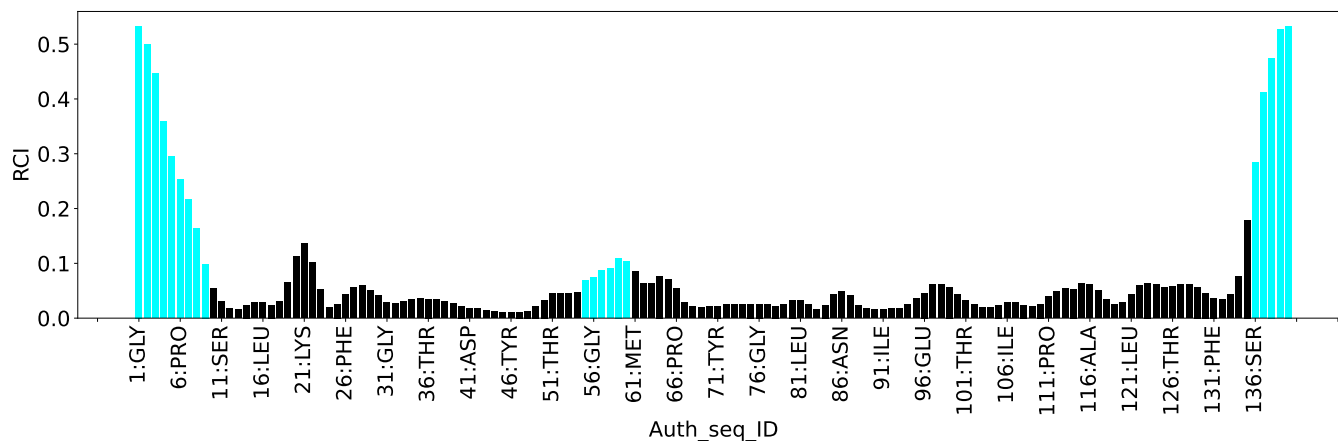
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	83	TYR	HA	1.62	1.87 – 7.33	-5.5
1	A	47	TYR	HD1	5.43	5.49 – 8.39	-5.2
1	A	47	TYR	HD2	5.43	5.48 – 8.39	-5.2
1	A	24	LEU	HD21	-0.67	-0.65 – 2.13	-5.1
1	A	24	LEU	HD22	-0.67	-0.65 – 2.13	-5.1
1	A	24	LEU	HD23	-0.67	-0.65 – 2.13	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	17
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	17
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.7	0.2
0.2-0.5 (Medium)	1.3	0.49
>0.5 (Large)	12.4	11.07

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

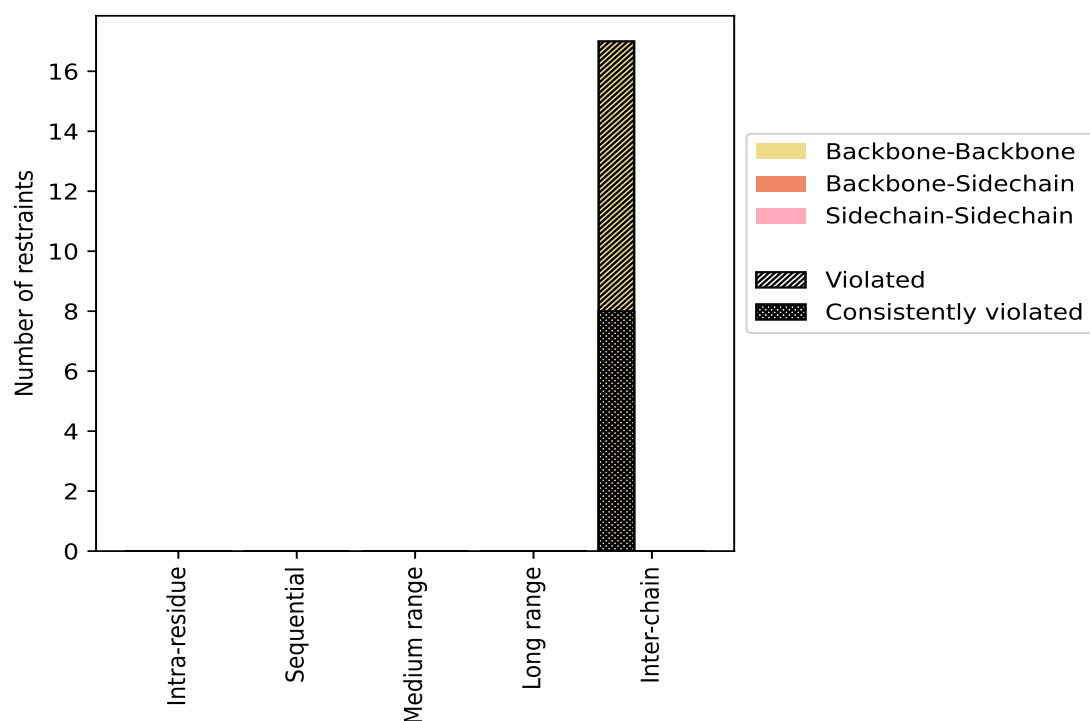
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	17	100.0	17	100.0	100.0	8	47.1	47.1
Backbone-Backbone	17	100.0	17	100.0	100.0	8	47.1	47.1
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	17	100.0	17	100.0	100.0	8	47.1	47.1
Backbone-Backbone	17	100.0	17	100.0	100.0	8	47.1	47.1
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfide bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	14	14	3.3	8.91	2.29	2.88
2	0	0	0	0	13	13	3.64	8.33	2.08	3.88
3	0	0	0	0	10	10	4.31	7.78	2.05	4.48
4	0	0	0	0	14	14	3.12	8.42	2.63	3.19
5	0	0	0	0	12	12	3.86	9.35	2.53	3.41
6	0	0	0	0	15	15	3.89	8.43	2.4	3.9
7	0	0	0	0	14	14	2.93	8.28	2.54	2.76
8	0	0	0	0	15	15	3.32	9.04	2.57	3.76
9	0	0	0	0	14	14	3.58	8.87	2.46	3.6
10	0	0	0	0	16	16	3.43	9.31	2.65	3.22

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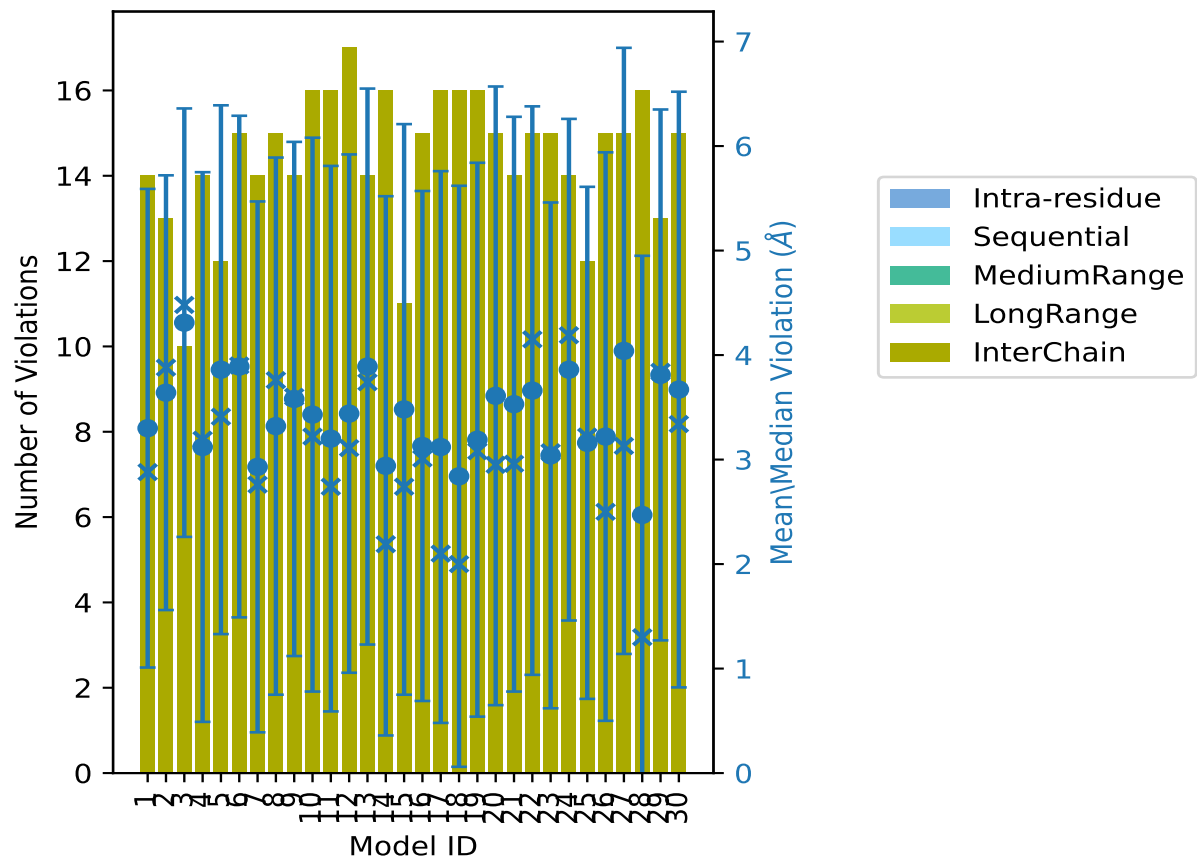
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	16	16	3.2	8.69	2.61	2.74
12	0	0	0	0	17	17	3.44	9.5	2.48	3.11
13	0	0	0	0	14	14	3.89	9.97	2.66	3.74
14	0	0	0	0	16	16	2.94	7.9	2.58	2.19
15	0	0	0	0	11	11	3.48	8.44	2.73	2.74
16	0	0	0	0	15	15	3.13	8.58	2.44	3.01
17	0	0	0	0	16	16	3.12	9.04	2.64	2.1
18	0	0	0	0	16	16	2.84	10.0	2.78	2.0
19	0	0	0	0	16	16	3.19	8.46	2.65	3.08
20	0	0	0	0	15	15	3.61	11.07	2.96	2.95
21	0	0	0	0	14	14	3.53	10.24	2.75	2.96
22	0	0	0	0	15	15	3.66	8.51	2.72	4.15
23	0	0	0	0	15	15	3.04	9.02	2.42	3.07
24	0	0	0	0	14	14	3.86	8.68	2.4	4.19
25	0	0	0	0	12	12	3.16	7.46	2.45	3.22
26	0	0	0	0	15	15	3.22	9.47	2.72	2.5
27	0	0	0	0	15	15	4.04	11.02	2.9	3.13
28	0	0	0	0	16	16	2.47	8.16	2.48	1.3
29	0	0	0	0	13	13	3.81	8.79	2.54	3.84
30	0	0	0	0	15	15	3.67	10.34	2.85	3.34

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	1	1	1	3.3
0	0	0	0	0	0	2	6.7
0	0	0	0	0	0	3	10.0
0	0	0	0	0	0	4	13.3
0	0	0	0	0	0	5	16.7
0	0	0	0	0	0	6	20.0

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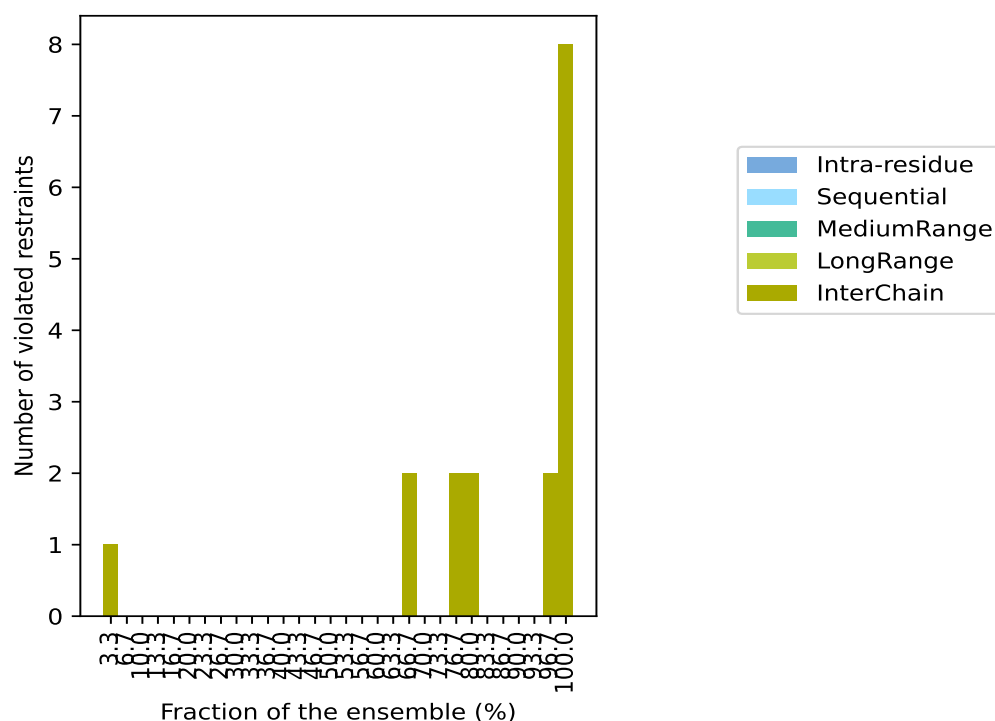
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	2	2	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	2	2	23	76.7
0	0	0	0	2	2	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	2	2	29	96.7
0	0	0	0	8	8	30	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

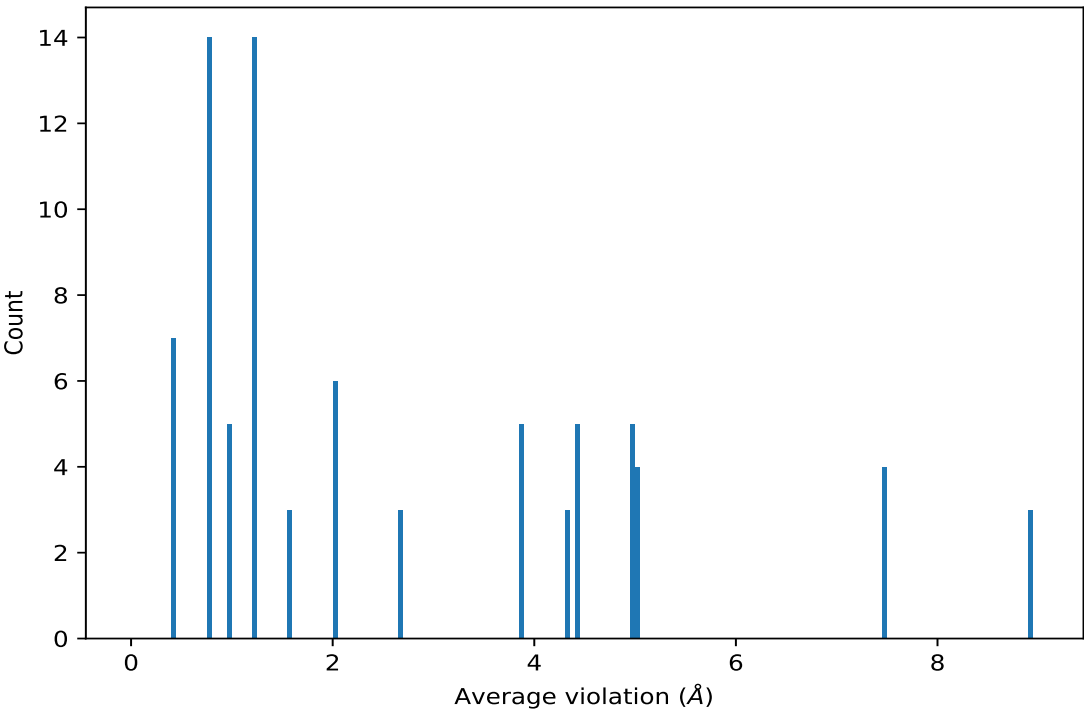
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	30	8.95	0.92	8.83
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	30	8.95	0.92	8.83
(1,1)	1:10:A:ALA:HB2	2:7:B:C:O2	30	8.95	0.92	8.83
(1,8)	1:109:A:ARG:HH21	2:7:B:C:O2	30	7.48	0.84	7.61
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	30	7.48	0.84	7.61
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	30	7.48	0.84	7.61
(1,8)	1:109:A:ARG:HH22	2:7:B:C:H41	30	7.48	0.84	7.61
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	30	5.03	0.44	5.04
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H5	30	5.03	0.44	5.04
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	30	5.03	0.44	5.04
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H42	30	5.03	0.44	5.04
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	30	4.99	0.54	4.81
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	30	4.99	0.54	4.81
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB1	30	4.99	0.54	4.81
(1,16)	2:6:B:A:H61	1:62:A:LYS:HZ1	30	4.99	0.54	4.81
(1,16)	2:6:B:A:H61	1:62:A:LYS:HZ2	30	4.99	0.54	4.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5)	1:54:A:ILE:HD13	2:2:B:A:H61	30	4.42	0.6	4.38
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	30	4.42	0.6	4.38
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	30	4.42	0.6	4.38
(1,5)	1:54:A:ILE:HD13	2:1:B:C:H42	30	4.42	0.6	4.38
(1,5)	1:54:A:ILE:HD11	2:1:B:C:H42	30	4.42	0.6	4.38
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	30	4.32	0.65	4.44
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ3	30	4.32	0.65	4.44
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	30	4.32	0.65	4.44
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	30	3.87	1.01	4.12
(1,3)	1:19:A:HIS:HB2	2:1:B:C:H5'	30	3.87	1.01	4.12
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H1'	30	3.87	1.01	4.12
(1,3)	1:19:A:HIS:HE1	2:1:B:C:H4'	30	3.87	1.01	4.12
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H4'	30	3.87	1.01	4.12
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	30	2.68	0.66	2.78
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	30	2.68	0.66	2.78
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	30	2.68	0.66	2.78
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	29	2.05	1.24	2.07
(1,6)	1:65:A:SER:OG	2:1:B:C:H5'	29	2.05	1.24	2.07
(1,6)	1:65:A:SER:H	2:1:B:C:H5	29	2.05	1.24	2.07
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	29	2.05	1.24	2.07
(1,6)	1:65:A:SER:H	2:1:B:C:H6	29	2.05	1.24	2.07
(1,6)	1:65:A:SER:OG	2:1:B:C:O4'	29	2.05	1.24	2.07
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	29	0.97	0.4	0.79
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	29	0.97	0.4	0.79
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ2	29	0.97	0.4	0.79
(1,13)	2:3:B:C:H42	1:62:A:LYS:HZ1	29	0.97	0.4	0.79
(1,13)	2:3:B:C:H41	1:62:A:LYS:HE3	29	0.97	0.4	0.79
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:HB1	2:7:B:C:H2'	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:O	2:7:B:C:H2'	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:O	2:7:B:C:HO2'	24	1.22	0.84	0.82
(1,9)	1:112:A:ALA:O	2:7:B:C:O2	24	1.22	0.84	0.82
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	24	1.22	0.84	0.82
(1,17)	2:7:B:C:H2'	1:112:A:ALA:HB1	24	1.22	0.84	0.82
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	24	1.22	0.84	0.82
(1,17)	2:7:B:C:H2'	1:112:A:ALA:O	24	1.22	0.84	0.82
(1,17)	2:7:B:C:O2	1:112:A:ALA:HB1	24	1.22	0.84	0.82
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:O	24	1.22	0.84	0.82
(1,17)	2:7:B:C:O2	1:112:A:ALA:O	24	1.22	0.84	0.82
(1,2)	1:17:A:THR:HG21	2:1:B:C:OP1	23	1.55	1.15	1.78

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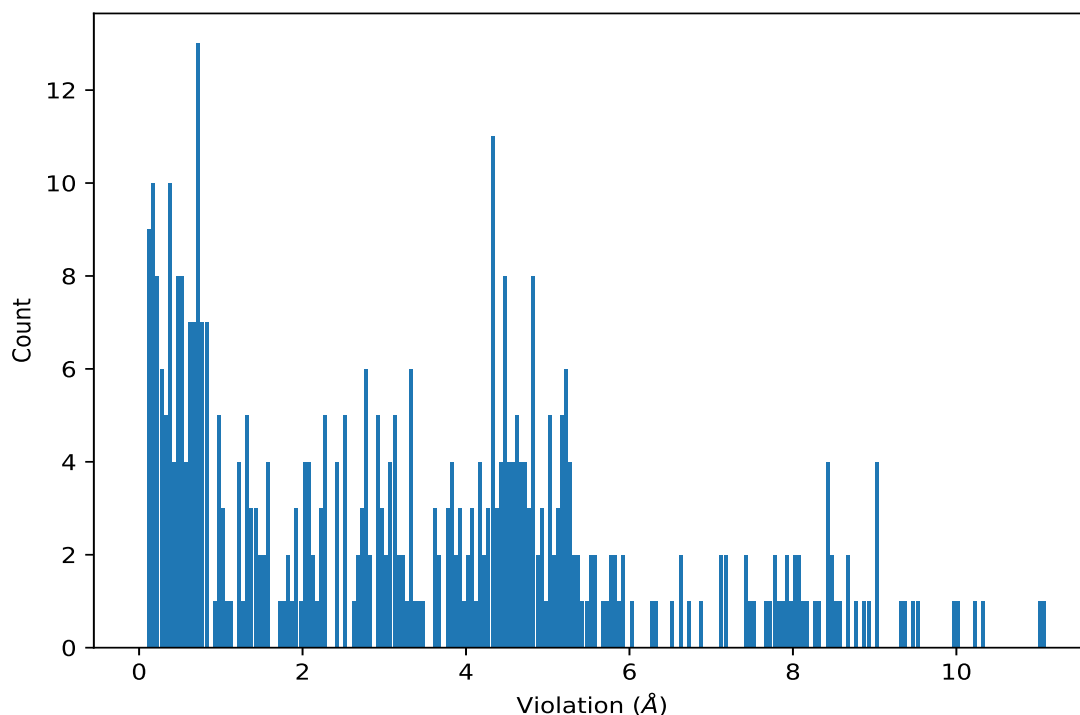
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	23	1.55	1.15	1.78
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	23	1.55	1.15	1.78
(1,12)	2:2:B:A:H62	1:62:A:LYS:HZ3	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H62	1:62:A:LYS:HE3	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ2	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ1	23	0.4	0.21	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HG3	23	0.4	0.21	0.38
(1,7)	1:67:A:ARG:HH21	2:1:B:C:OP1	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HE	2:1:B:C:OP1	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HE	2:1:B:C:HOP3	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HH21	2:1:B:C:O5'	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HH12	2:1:B:C:HOP3	20	0.76	0.85	0.41
(1,7)	1:67:A:ARG:HD2	2:1:B:C:HOP3	20	0.76	0.85	0.41
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	20	0.75	0.74	0.52
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5'	20	0.75	0.74	0.52
(1,10)	1:132:A:TYR:OH	2:1:B:C:H5'	20	0.75	0.74	0.52
(1,10)	1:132:A:TYR:HH	2:1:B:C:H5'	20	0.75	0.74	0.52
(1,10)	1:132:A:TYR:HE1	2:1:B:C:OP1	20	0.75	0.74	0.52
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5''	20	0.75	0.74	0.52

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	20	11.07
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	27	11.02
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	30	10.34
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	21	10.24
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	18	10.0
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	13	9.97
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	12	9.5
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	26	9.47
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	5	9.35
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	10	9.31
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	8	9.04
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	17	9.04
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	23	9.02
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	27	9.0
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	1	8.91
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	9	8.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	29	8.79
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	11	8.69
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	24	8.68
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	16	8.58
(1,8)	1:109:A:ARG:HH22	2:7:B:C:H41	22	8.51
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	19	8.46
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	19	8.45
(1,1)	1:10:A:ALA:HB2	2:7:B:C:O2	15	8.44
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	6	8.43
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	4	8.42
(1,1)	1:10:A:ALA:HB2	2:7:B:C:O2	22	8.4
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	2	8.33
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	7	8.28
(1,1)	1:10:A:ALA:HB1	2:7:B:C:O2	28	8.16
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	20	8.14
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	15	8.09
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	30	8.09
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	29	8.03
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	13	8.0
(1,1)	1:10:A:ALA:HB2	2:7:B:C:O2	4	7.95
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	6	7.93
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	14	7.9
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	21	7.89
(1,8)	1:109:A:ARG:HH22	2:7:B:C:H41	26	7.8
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	10	7.78
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	3	7.78
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	17	7.72
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	11	7.65
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	12	7.5
(1,1)	1:10:A:ALA:HB3	2:7:B:C:O2	25	7.46
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	24	7.41
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	25	7.4
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	14	7.15
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	18	7.15
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	8	7.14
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	16	7.11
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	7	6.89
(1,8)	1:109:A:ARG:HH22	2:7:B:C:O2	3	6.72
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	5	6.61
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	9	6.61
(1,8)	1:109:A:ARG:HH12	2:7:B:C:O2	23	6.54
(1,8)	1:109:A:ARG:HH21	2:7:B:C:O2	1	6.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	2:6:B:A:H61	1:62:A:LYS:HZ2	27	6.27
(1,8)	1:109:A:ARG:HH21	2:7:B:C:O2	28	6.02
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	30	5.91
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	5	5.91
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	6	5.85
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	6	5.83
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	22	5.8
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H5	22	5.79
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	9	5.78
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB1	20	5.74
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	13	5.68
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	17	5.58
(1,16)	2:6:B:A:H61	1:62:A:LYS:HZ1	26	5.55
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	5	5.53
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	8	5.53
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB1	29	5.45
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H42	10	5.43
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	11	5.39
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	9	5.37
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	14	5.33
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	6	5.3
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	7	5.29
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	14	5.28
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	24	5.26
(1,8)	1:109:A:ARG:HH21	2:7:B:C:O2	2	5.25
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	3	5.24
(1,5)	1:54:A:ILE:HD13	2:1:B:C:H42	22	5.21
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	12	5.21
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	22	5.2
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	3	5.2
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	2	5.2
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	12	5.19
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	21	5.18
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	24	5.16
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H42	27	5.16
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	19	5.15
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H5	2	5.14
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	14	5.13
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	11	5.12
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	28	5.07
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	10	5.06
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	30	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	14	5.03
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	20	5.01
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	18	5.0
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	13	5.0
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	13	4.99
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	3	4.93
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H5	29	4.93
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	16	4.91
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	15	4.87
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H42	30	4.86
(1,5)	1:54:A:ILE:HD11	2:1:B:C:H42	28	4.84
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	30	4.84
(1,3)	1:19:A:HIS:HB2	2:1:B:C:H5'	27	4.84
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	4	4.83
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	10	4.82
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	18	4.82
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	26	4.82
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	10	4.8
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	29	4.79
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	17	4.78
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	11	4.76
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	23	4.73
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	15	4.73
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	19	4.73
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	9	4.7
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	1	4.68
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	24	4.68
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	27	4.68
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	16	4.67
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	12	4.64
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	1	4.64
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	8	4.63
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	28	4.63
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	24	4.62
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	25	4.58
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	4	4.57
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	20	4.55
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	13	4.55
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	11	4.51
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	7	4.51
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	19	4.51
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	12	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	19	4.49
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	17	4.47
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	10	4.45
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	21	4.45
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	23	4.45
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	21	4.45
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ3	27	4.45
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	30	4.45
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	29	4.43
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	2	4.42
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	5	4.42
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	15	4.42
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	8	4.39
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	6	4.38
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	20	4.38
(1,16)	2:6:B:A:H2	1:112:A:ALA:HB3	16	4.34
(1,4)	1:52:A:ARG:O	2:1:B:C:H42	25	4.34
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	8	4.34
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	17	4.33
(1,16)	2:6:B:A:H2	1:112:A:ALA:HA	9	4.32
(1,4)	1:52:A:ARG:HB3	2:1:B:C:H5	23	4.32
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	21	4.31
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	22	4.3
(1,5)	1:54:A:ILE:HD13	2:2:B:A:H61	19	4.3
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	11	4.3
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	24	4.3
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	17	4.28
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	12	4.26
(1,6)	1:65:A:SER:H	2:1:B:C:H5	6	4.26
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	25	4.23
(1,5)	1:54:A:ILE:HD13	2:2:B:A:H61	1	4.2
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	9	4.19
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	4	4.17
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H1'	13	4.15
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	22	4.15
(1,6)	1:65:A:SER:OG	2:1:B:C:H5'	2	4.12
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	26	4.08
(1,6)	1:65:A:SER:H	2:1:B:C:H5	24	4.07
(1,4)	1:52:A:ARG:O	2:1:B:C:H5	16	4.06
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	18	4.04
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ3	3	4.03
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	1	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	5	3.92
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	23	3.91
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	6	3.9
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	2	3.88
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	18	3.85
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	7	3.84
(1,6)	1:65:A:SER:H	2:1:B:C:H5	8	3.84
(1,3)	1:19:A:HIS:HB2	2:1:B:C:H5'	29	3.84
(1,3)	1:19:A:HIS:HB2	2:1:B:C:H5'	3	3.8
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	7	3.79
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	26	3.78
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	8	3.76
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	6	3.67
(1,5)	1:54:A:ILE:HD12	2:2:B:A:H61	26	3.65
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	4	3.64
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	24	3.6
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	4	3.6
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	10	3.47
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	18	3.41
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	14	3.37
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	13	3.34
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	30	3.34
(1,6)	1:65:A:SER:H	2:1:B:C:H6	19	3.34
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	12	3.33
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	25	3.32
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	7	3.3
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	2	3.26
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ1	28	3.23
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	24	3.23
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	21	3.16
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	23	3.15
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	27	3.13
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	27	3.13
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ3	25	3.11
(1,7)	1:67:A:ARG:HE	2:1:B:C:HOP3	12	3.11
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	1	3.1
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	23	3.07
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	11	3.06
(1,5)	1:54:A:ILE:HD11	2:2:B:A:H61	16	3.06
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	12	3.05
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	9	3.01
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	16	3.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	10	2.98
(1,17)	2:7:B:C:O2	1:112:A:ALA:O	20	2.95
(1,9)	1:112:A:ALA:O	2:7:B:C:O2	20	2.95
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	2	2.93
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	12	2.93
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	20	2.91
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	29	2.9
(1,6)	1:65:A:SER:OG	2:1:B:C:H5'	5	2.9
(1,10)	1:132:A:TYR:HE1	2:1:B:C:OP1	16	2.82
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	19	2.81
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	4	2.78
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H4'	20	2.78
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	8	2.78
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	10	2.78
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	21	2.77
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	28	2.76
(1,15)	2:5:B:G:O6	1:62:A:LYS:HZ2	15	2.74
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	27	2.74
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	17	2.72
(1,6)	1:65:A:SER:H	2:1:B:C:H5	3	2.67
(1,7)	1:67:A:ARG:HH21	2:1:B:C:OP1	1	2.66
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	18	2.62
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	9	2.54
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	6	2.53
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	5	2.51
(1,17)	2:7:B:C:H2'	1:112:A:ALA:HB1	26	2.5
(1,9)	1:112:A:ALA:HB1	2:7:B:C:H2'	26	2.5
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	1	2.44
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	22	2.44
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	11	2.43
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5'	6	2.4
(1,17)	2:7:B:C:O2	1:112:A:ALA:HB1	13	2.29
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	5	2.29
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2	13	2.29
(1,6)	1:65:A:SER:OG	2:1:B:C:O4'	20	2.28
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	14	2.26
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	3	2.22
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	7	2.21
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	21	2.21
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	11	2.19
(1,3)	1:19:A:HIS:HD1	2:1:B:C:H5'	14	2.13
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	2	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:7:B:C:O2	1:112:A:ALA:HB1	29	2.08
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2	29	2.08
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	26	2.07
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	27	2.07
(1,2)	1:17:A:THR:HG21	2:1:B:C:OP1	5	2.04
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	8	2.01
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	30	2.0
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	30	2.0
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	22	1.98
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	13	1.94
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	27	1.93
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	9	1.91
(1,2)	1:17:A:THR:HG21	2:1:B:C:OP1	1	1.86
(1,2)	1:17:A:THR:OG1	2:1:B:C:OP1	16	1.81
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ1	28	1.8
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	21	1.78
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	12	1.71
(1,6)	1:65:A:SER:H	2:1:B:C:H5	15	1.59
(1,17)	2:7:B:C:H2'	1:112:A:ALA:HB1	6	1.58
(1,9)	1:112:A:ALA:HB1	2:7:B:C:H2'	6	1.58
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	1	1.58
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	2	1.54
(1,7)	1:67:A:ARG:HD2	2:1:B:C:HOP3	23	1.53
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	17	1.48
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	17	1.48
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	30	1.43
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ3	25	1.41
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	13	1.41
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ2	18	1.39
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	30	1.36
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	4	1.35
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	23	1.34
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	24	1.33
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	14	1.32
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	19	1.31
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	19	1.31
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5''	17	1.28
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:O	12	1.24
(1,9)	1:112:A:ALA:O	2:7:B:C:HO2'	12	1.24
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	29	1.23
(1,10)	1:132:A:TYR:HE1	2:1:B:C:OP1	23	1.22
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	9	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	11	1.05
(1,2)	1:17:A:THR:HG21	2:1:B:C:OP1	4	1.03
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	27	1.03
(1,3)	1:19:A:HIS:HE1	2:1:B:C:H4'	15	1.02
(1,17)	2:7:B:C:O2	1:112:A:ALA:HB1	21	0.97
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2	21	0.97
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	25	0.97
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ2	10	0.96
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ2	21	0.96
(1,14)	2:4:B:U:O4	1:62:A:LYS:HZ2	15	0.94
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	23	0.84
(1,17)	2:7:B:C:H2'	1:112:A:ALA:HB1	22	0.83
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	9	0.83
(1,9)	1:112:A:ALA:HB1	2:7:B:C:H2'	22	0.83
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	12	0.82
(1,17)	2:7:B:C:O2	1:112:A:ALA:HB1	10	0.8
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2	10	0.8
(1,17)	2:7:B:C:H2'	1:112:A:ALA:O	8	0.79
(1,13)	2:3:B:C:H42	1:62:A:LYS:HZ1	16	0.79
(1,13)	2:3:B:C:H41	1:62:A:LYS:HE3	28	0.79
(1,9)	1:112:A:ALA:O	2:7:B:C:H2'	8	0.79
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	22	0.77
(1,13)	2:3:B:C:H42	1:62:A:LYS:HZ1	27	0.76
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	17	0.75
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	1	0.74
(1,13)	2:3:B:C:H42	1:62:A:LYS:HZ1	20	0.74
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	24	0.73
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	24	0.73
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	17	0.73
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	19	0.72
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	18	0.72
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	15	0.71
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	18	0.71
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	15	0.71
(1,17)	2:7:B:C:H2'	1:112:A:ALA:O	23	0.7
(1,9)	1:112:A:ALA:O	2:7:B:C:H2'	23	0.7
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	4	0.7
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	9	0.69
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	10	0.69
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	7	0.68
(1,13)	2:3:B:C:H42	1:62:A:LYS:HZ1	17	0.68
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	30	0.66
(1,10)	1:132:A:TYR:OH	2:1:B:C:H5'	7	0.65
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	14	0.63
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	7	0.62
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ1	22	0.62
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	7	0.62
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	26	0.61
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ2	11	0.61
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	2	0.6
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	1	0.59
(1,10)	1:132:A:TYR:OH	2:1:B:C:H5'	10	0.58
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5''	26	0.58
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	13	0.55
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	16	0.54
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:O	18	0.54
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	16	0.54
(1,9)	1:112:A:ALA:O	2:7:B:C:HO2'	18	0.54
(1,6)	1:65:A:SER:HG	2:1:B:C:O4'	29	0.53
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	2	0.52
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	5	0.51
(1,12)	2:2:B:A:H62	1:62:A:LYS:HZ3	1	0.51
(1,12)	2:2:B:A:H61	1:62:A:LYS:HG3	28	0.49
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	26	0.49
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	3	0.47
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ1	8	0.47
(1,10)	1:132:A:TYR:OH	2:1:B:C:H5'	25	0.47
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	16	0.47
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	11	0.46
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	19	0.45
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	14	0.43
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	14	0.43
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	29	0.41
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	30	0.4
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	11	0.39
(1,17)	2:7:B:C:O2'	1:112:A:ALA:HB1	28	0.39
(1,10)	1:132:A:TYR:HH	2:1:B:C:H5'	19	0.39
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	11	0.39
(1,9)	1:112:A:ALA:HB1	2:7:B:C:O2'	28	0.39
(1,12)	2:2:B:A:H62	1:62:A:LYS:HE3	4	0.38
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	17	0.38
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	13	0.37
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5'	27	0.35
(1,12)	2:2:B:A:H62	1:62:A:LYS:HE3	25	0.33
(1,13)	2:3:B:C:H41	1:62:A:LYS:HZ3	25	0.32
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	14	0.32
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	19	0.31
(1,7)	1:67:A:ARG:HH21	2:1:B:C:O5'	20	0.31
(1,10)	1:132:A:TYR:HH	2:1:B:C:H5'	30	0.29
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	28	0.27
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	18	0.26
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	7	0.25
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	17	0.25
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	19	0.25
(1,7)	1:67:A:ARG:HH21	2:1:B:C:OP1	26	0.24
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	28	0.24
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	16	0.23
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	24	0.23
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	9	0.22
(1,6)	1:65:A:SER:HG	2:1:B:C:H5'	18	0.21
(1,7)	1:67:A:ARG:HH21	2:1:B:C:OP1	28	0.2
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	28	0.2
(1,12)	2:2:B:A:H62	1:62:A:LYS:HE3	8	0.17
(1,10)	1:132:A:TYR:HH	2:1:B:C:H5'	14	0.17
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	8	0.17
(1,7)	1:67:A:ARG:HH21	2:1:B:C:HOP3	14	0.17
(1,17)	2:7:B:C:HO2'	1:112:A:ALA:HB1	4	0.16
(1,10)	1:132:A:TYR:OH	2:1:B:C:H5'	11	0.16
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	18	0.16
(1,9)	1:112:A:ALA:HB1	2:7:B:C:HO2'	4	0.16
(1,12)	2:2:B:A:H61	1:62:A:LYS:HZ3	20	0.15
(1,10)	1:132:A:TYR:HE1	2:1:B:C:H5'	20	0.15
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	21	0.14
(1,11)	2:1:B:C:OP1	1:132:A:TYR:HH	12	0.14
(1,10)	1:132:A:TYR:HH	2:1:B:C:OP1	12	0.14
(1,7)	1:67:A:ARG:HE	2:1:B:C:OP1	7	0.14
(1,2)	1:17:A:THR:HG1	2:1:B:C:OP1	23	0.14
(1,12)	2:2:B:A:H61	1:62:A:LYS:HE3	10	0.13
(1,12)	2:2:B:A:H62	1:62:A:LYS:HE3	26	0.13
(1,7)	1:67:A:ARG:HH22	2:1:B:C:HOP3	6	0.12
(1,7)	1:67:A:ARG:HH12	2:1:B:C:HOP3	22	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found