



Full wwPDB NMR Structure Validation Report ⓘ

Oct 19, 2020 – 11:06 AM BST

PDB ID : 7ACT
Title : The SARS-CoV-2 nucleocapsid phosphoprotein N-terminal domain in complex with 10mer ssRNA
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.14.6
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

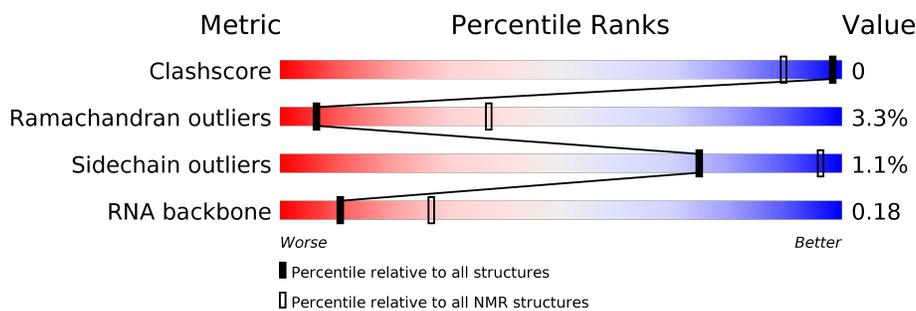
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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	10	

2 Ensemble composition and analysis i

This entry contains 10 models. Model 5 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:46-A:95, A:102-A:174 (123)	0.45	5

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 2 single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 8
2	3, 4
3	9, 10
Single-model clusters	1; 2

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2390 atoms, of which 1128 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	137	2072	661	1020	192	198	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLY	-	expression tag	UNP P0DTC9
A	42	ALA	-	expression tag	UNP P0DTC9
A	43	MET	-	expression tag	UNP P0DTC9

- Molecule 2 is a RNA chain called ssRNA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	10	318	94	108	35	71	10	0

4 Residue-property plots [i](#)

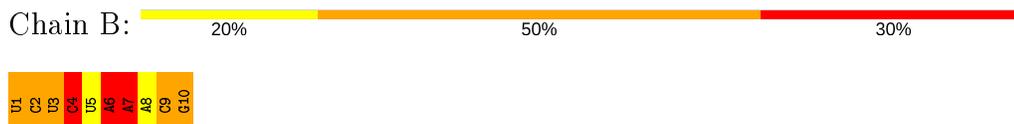
4.1 Average score per residue in the NMR ensemble

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: ssRNA

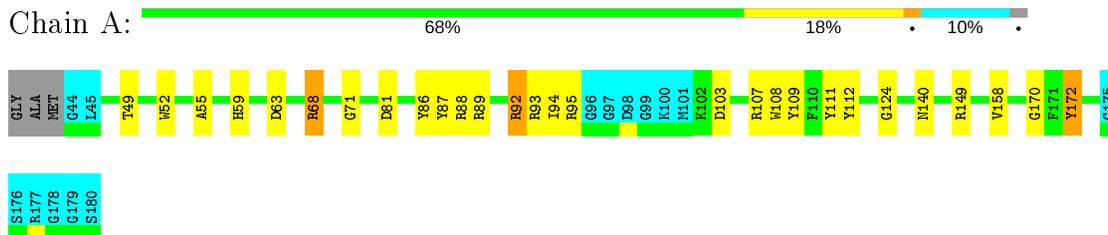


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Nucleoprotein



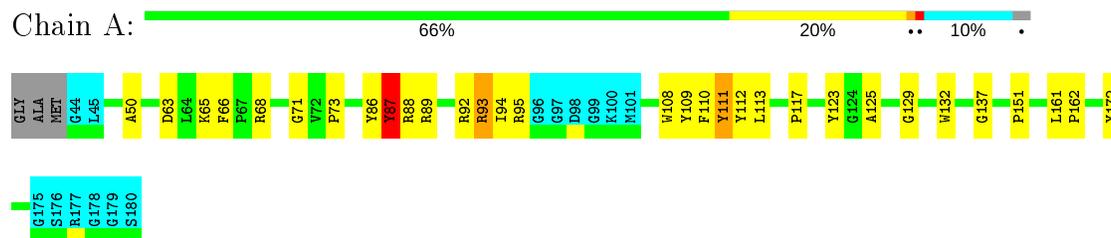
- Molecule 2: ssRNA



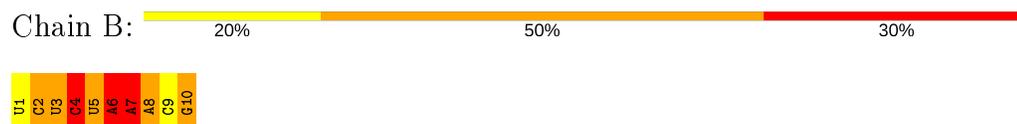


4.2.2 Score per residue for model 2

- Molecule 1: Nucleoprotein

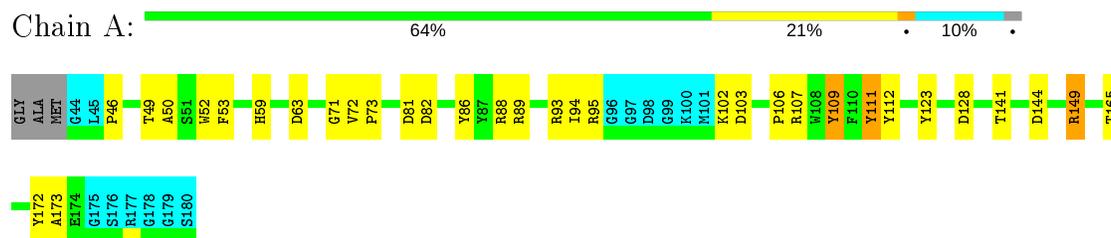


- Molecule 2: ssRNA

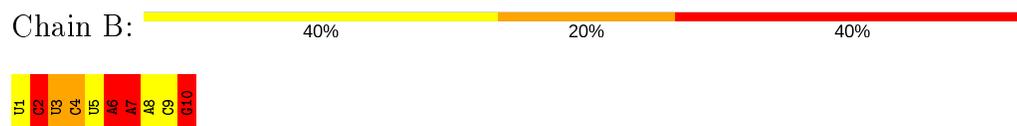


4.2.3 Score per residue for model 3

- Molecule 1: Nucleoprotein



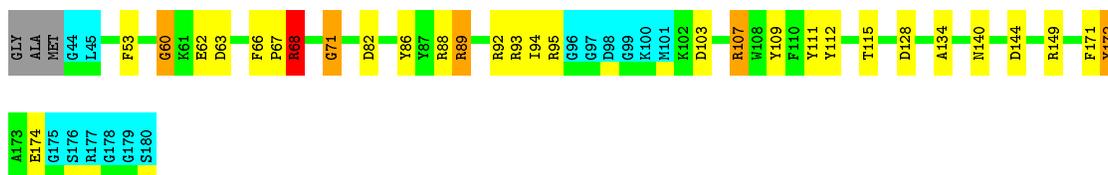
- Molecule 2: ssRNA



4.2.4 Score per residue for model 4

- Molecule 1: Nucleoprotein



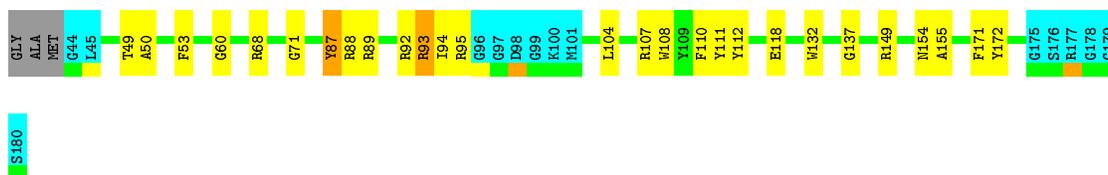


- Molecule 2: ssRNA



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Nucleoprotein



- Molecule 2: ssRNA



4.2.6 Score per residue for model 6

- Molecule 1: Nucleoprotein



- Molecule 2: ssRNA





4.2.7 Score per residue for model 7

- Molecule 1: Nucleoprotein

Chain A: 71% 16% 10%



- Molecule 2: ssRNA

Chain B: 10% 50% 40%



4.2.8 Score per residue for model 8

- Molecule 1: Nucleoprotein

Chain A: 66% 20% 10%



- Molecule 2: ssRNA

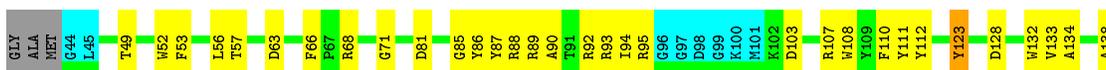
Chain B: 40% 30% 30%



4.2.9 Score per residue for model 9

- Molecule 1: Nucleoprotein

Chain A: 64% 24% 10%



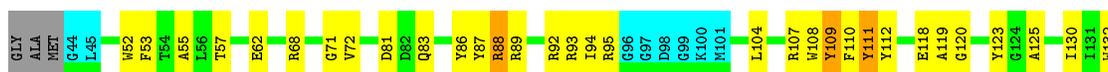


- Molecule 2: ssRNA



4.2.10 Score per residue for model 10

- Molecule 1: Nucleoprotein



- Molecule 2: ssRNA



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
YASARA	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%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1.59±0.03	6±2/997 (0.6± 0.2%)	1.99±0.07	30±5/1361 (2.2± 0.3%)
2	B	3.05±0.18	22±5/233 (9.4± 2.3%)	3.77±0.25	60±9/358 (16.7± 2.4%)
All	All	1.95	275/12300 (2.2%)	2.48	897/17190 (5.2%)

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	Planarity
1	A	0.0±0.0	3.4±1.4
2	B	2.0±0.0	5.3±1.0
All	All	20	87

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
2	B	6	A	N9-C4	-14.96	1.28	1.37	4	4
2	B	1	U	OP3-P	-14.40	1.43	1.61	3	10
2	B	8	A	N7-C5	14.07	1.47	1.39	10	4
2	B	9	C	C4-N4	-11.15	1.24	1.33	10	4
2	B	9	C	N3-C4	-10.88	1.26	1.33	9	2
2	B	8	A	C6-N6	-10.32	1.25	1.33	5	3
2	B	10	G	N1-C2	-9.86	1.29	1.37	1	1
2	B	7	A	P-O5'	9.85	1.69	1.59	7	3
2	B	1	U	C5'-C4'	9.80	1.63	1.51	7	1
2	B	8	A	C6-N1	-9.79	1.28	1.35	1	4
2	B	2	C	N3-C4	-9.69	1.27	1.33	9	3
2	B	9	C	C5'-C4'	9.49	1.62	1.51	4	1
2	B	3	U	C2-N3	-9.46	1.31	1.37	4	1
2	B	1	U	O3'-P	-9.29	1.50	1.61	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	6	A	P-O5'	9.24	1.69	1.59	3	4
2	B	8	A	N9-C4	8.95	1.43	1.37	7	1
2	B	1	U	C4-C5	8.85	1.51	1.43	4	1
2	B	6	A	C5'-C4'	8.72	1.61	1.51	2	2
2	B	4	C	N3-C4	-8.72	1.27	1.33	2	3
2	B	9	C	C5-C6	8.37	1.41	1.34	10	3
2	B	6	A	C6-N1	-8.35	1.29	1.35	5	1
2	B	7	A	N7-C5	8.32	1.44	1.39	2	4
2	B	3	U	O3'-P	-8.18	1.51	1.61	1	1
2	B	5	U	C4-C5	8.16	1.50	1.43	4	3
2	B	7	A	N3-C4	8.14	1.39	1.34	1	1
2	B	6	A	C6-N6	-8.11	1.27	1.33	1	1
2	B	9	C	C4'-O4'	-8.05	1.35	1.45	5	2
2	B	8	A	N1-C2	-8.03	1.27	1.34	7	3
2	B	8	A	P-O5'	8.02	1.67	1.59	6	1
2	B	2	C	N1-C6	8.01	1.42	1.37	5	1
1	A	67	PRO	N-CD	-7.95	1.36	1.47	4	1
2	B	10	G	C2'-O2'	7.90	1.51	1.41	6	1
2	B	1	U	P-O5'	-7.79	1.51	1.59	3	2
2	B	5	U	P-O5'	-7.78	1.51	1.59	4	2
2	B	4	C	P-O5'	7.76	1.67	1.59	3	1
2	B	6	A	C4'-O4'	-7.62	1.35	1.45	1	1
2	B	9	C	O3'-P	-7.58	1.52	1.61	5	2
2	B	9	C	N1-C6	7.56	1.41	1.37	9	1
2	B	10	G	C2-N2	-7.55	1.26	1.34	7	2
1	A	88	ARG	CZ-NH1	-7.54	1.23	1.33	8	1
2	B	3	U	C3'-C2'	7.53	1.61	1.52	8	2
2	B	8	A	N3-C4	7.53	1.39	1.34	5	3
2	B	5	U	N1-C6	7.34	1.44	1.38	2	3
2	B	7	A	C2'-C1'	7.33	1.61	1.53	10	1
2	B	3	U	C5-C6	7.27	1.40	1.34	4	1
2	B	9	C	C2'-C1'	-7.25	1.45	1.53	6	1
2	B	8	A	N9-C8	7.23	1.43	1.37	3	6
2	B	2	C	C3'-O3'	-7.19	1.32	1.42	7	1
2	B	10	G	N9-C4	7.16	1.43	1.38	4	1
2	B	6	A	N9-C8	-7.16	1.32	1.37	3	4
2	B	6	A	N7-C5	7.16	1.43	1.39	10	2
1	A	93	ARG	CZ-NH1	-7.15	1.23	1.33	10	1
2	B	4	C	C4-C5	-7.14	1.37	1.43	5	2
2	B	3	U	C4-C5	7.11	1.50	1.43	5	2
2	B	7	A	C2'-O2'	7.06	1.50	1.41	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	5	U	N1-C2	7.04	1.44	1.38	3	2
2	B	5	U	C2-N3	7.03	1.42	1.37	2	1
2	B	6	A	C8-N7	-7.00	1.26	1.31	4	1
2	B	10	G	C5-C6	6.95	1.49	1.42	10	2
2	B	6	A	C2'-C1'	-6.93	1.45	1.53	5	2
2	B	6	A	O4'-C1'	6.86	1.50	1.41	6	1
2	B	9	C	P-O5'	-6.80	1.52	1.59	10	2
1	A	92	ARG	CZ-NH2	-6.77	1.24	1.33	10	1
1	A	112	TYR	CG-CD2	6.69	1.47	1.39	10	1
2	B	7	A	C6-N1	-6.68	1.30	1.35	7	3
1	A	124	GLY	CA-C	6.66	1.62	1.51	1	1
2	B	10	G	O4'-C1'	6.66	1.50	1.41	9	1
1	A	129	GLY	CA-C	6.66	1.62	1.51	2	1
2	B	7	A	N9-C4	6.64	1.41	1.37	7	2
2	B	4	C	C4-N4	-6.63	1.27	1.33	7	3
2	B	8	A	C4'-C3'	-6.60	1.45	1.53	1	2
2	B	5	U	C3'-C2'	-6.60	1.45	1.52	1	1
2	B	2	C	C4'-C3'	6.59	1.60	1.53	6	2
2	B	4	C	C5-C6	6.58	1.39	1.34	7	1
2	B	5	U	N3-C4	6.56	1.44	1.38	10	1
2	B	5	U	C5-C6	6.50	1.40	1.34	9	3
2	B	10	G	P-O5'	6.50	1.66	1.59	1	1
2	B	3	U	N1-C6	-6.47	1.32	1.38	6	1
2	B	7	A	N9-C8	6.45	1.43	1.37	6	1
2	B	6	A	N3-C4	6.43	1.38	1.34	7	1
1	A	59	HIS	CB-CG	6.43	1.61	1.50	3	2
2	B	10	G	C5-C4	-6.41	1.33	1.38	1	1
2	B	10	G	C6-O6	6.40	1.29	1.24	6	2
2	B	2	C	C3'-C2'	6.39	1.59	1.52	7	1
2	B	6	A	C5-C6	6.37	1.46	1.41	2	2
1	A	172	TYR	CE2-CZ	6.25	1.46	1.38	7	1
1	A	109	TYR	CD1-CE1	6.24	1.48	1.39	10	1
1	A	93	ARG	CZ-NH2	-6.21	1.25	1.33	10	3
1	A	68	ARG	CZ-NH2	-6.19	1.25	1.33	7	1
2	B	1	U	C2'-O2'	6.18	1.49	1.41	9	1
2	B	7	A	C5-C4	-6.17	1.34	1.38	9	2
1	A	93	ARG	NE-CZ	6.16	1.41	1.33	1	1
1	A	118	GLU	CD-OE1	-6.13	1.19	1.25	6	1
2	B	5	U	C5'-C4'	6.10	1.58	1.51	3	1
2	B	3	U	C4-O4	-6.08	1.18	1.23	10	1
1	A	107	ARG	CZ-NH2	-6.06	1.25	1.33	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	172	TYR	CE1-CZ	6.05	1.46	1.38	3	3
2	B	4	C	N1-C2	6.04	1.46	1.40	10	2
1	A	109	TYR	CE1-CZ	6.04	1.46	1.38	7	1
2	B	8	A	C2-N3	-6.03	1.28	1.33	3	1
2	B	2	C	C4-C5	-6.03	1.38	1.43	5	2
1	A	60	GLY	CA-C	6.01	1.61	1.51	5	1
2	B	3	U	C4'-C3'	-6.00	1.46	1.52	2	1
1	A	68	ARG	CZ-NH1	-5.99	1.25	1.33	8	1
2	B	2	C	C5'-C4'	5.94	1.58	1.51	5	2
1	A	95	ARG	CZ-NH2	-5.94	1.25	1.33	2	3
2	B	1	U	C2'-C1'	5.92	1.59	1.53	7	1
2	B	4	C	C5'-C4'	5.91	1.58	1.51	3	3
2	B	8	A	C3'-C2'	5.89	1.59	1.52	1	2
2	B	4	C	C2-O2	5.89	1.29	1.24	9	1
1	A	172	TYR	CG-CD1	5.87	1.46	1.39	8	1
2	B	2	C	C2'-C1'	-5.86	1.47	1.53	3	1
2	B	3	U	C2'-C1'	5.84	1.59	1.53	5	1
2	B	7	A	C5-C6	5.80	1.46	1.41	8	2
2	B	5	U	C2'-C1'	5.78	1.59	1.53	2	2
2	B	9	C	C2'-O2'	5.78	1.49	1.41	7	2
2	B	10	G	C6-N1	-5.77	1.35	1.39	2	2
2	B	10	G	N3-C4	5.77	1.39	1.35	1	1
2	B	2	C	P-O5'	5.76	1.65	1.59	1	1
2	B	1	U	N3-C4	-5.74	1.33	1.38	10	2
2	B	10	G	C2-N3	5.68	1.37	1.32	4	2
2	B	3	U	O4'-C1'	5.68	1.49	1.41	6	1
2	B	4	C	C3'-C2'	5.67	1.59	1.52	5	1
2	B	7	A	C6-N6	-5.63	1.29	1.33	10	2
1	A	149	ARG	CZ-NH1	-5.62	1.25	1.33	10	1
2	B	2	C	C5-C6	-5.62	1.29	1.34	10	1
2	B	10	G	N7-C5	5.57	1.42	1.39	10	3
2	B	8	A	C5'-C4'	5.56	1.58	1.51	9	1
2	B	2	C	C4-N4	-5.55	1.28	1.33	10	2
2	B	4	C	O3'-P	-5.52	1.54	1.61	7	1
2	B	2	C	C2-N3	5.51	1.40	1.35	9	2
2	B	5	U	C4'-C3'	-5.47	1.47	1.52	6	1
2	B	1	U	N1-C2	5.46	1.43	1.38	10	1
2	B	6	A	O3'-P	-5.44	1.54	1.61	1	1
1	A	71	GLY	CA-C	5.43	1.60	1.51	4	1
2	B	5	U	C4'-O4'	-5.42	1.38	1.45	9	1
1	A	123	TYR	CE2-CZ	5.42	1.45	1.38	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	109	TYR	CG-CD1	5.41	1.46	1.39	2	1
2	B	1	U	C5-C6	5.41	1.39	1.34	2	2
1	A	147	GLY	CA-C	5.41	1.60	1.51	8	1
1	A	123	TYR	CG-CD1	5.40	1.46	1.39	10	1
1	A	62	GLU	CD-OE2	-5.39	1.19	1.25	4	1
1	A	92	ARG	CZ-NH1	-5.38	1.26	1.33	5	1
1	A	73	PRO	N-CD	-5.37	1.40	1.47	2	1
1	A	62	GLU	CG-CD	5.37	1.60	1.51	4	1
1	A	137	GLY	CA-C	5.34	1.60	1.51	5	2
2	B	3	U	C2-O2	5.34	1.27	1.22	8	1
1	A	149	ARG	NE-CZ	5.33	1.40	1.33	1	1
1	A	92	ARG	NE-CZ	5.29	1.40	1.33	4	1
1	A	89	ARG	NE-CZ	5.29	1.40	1.33	2	1
1	A	171	PHE	CG-CD1	5.27	1.46	1.38	5	1
2	B	3	U	N1-C2	5.26	1.43	1.38	10	1
2	B	7	A	C4'-O4'	-5.25	1.38	1.45	8	1
2	B	6	A	C5-C4	-5.24	1.35	1.38	6	1
2	B	7	A	C4'-C3'	-5.24	1.47	1.52	4	1
1	A	78	SER	CB-OG	-5.21	1.35	1.42	8	1
1	A	170	GLY	CA-C	5.15	1.60	1.51	1	1
1	A	172	TYR	CG-CD2	5.14	1.45	1.39	2	2
1	A	112	TYR	CG-CD1	5.13	1.45	1.39	4	1
1	A	132	TRP	CD2-CE2	5.13	1.47	1.41	5	1
1	A	118	GLU	N-CA	5.12	1.56	1.46	7	1
1	A	51	SER	CB-OG	5.11	1.48	1.42	8	1
1	A	107	ARG	CZ-NH1	-5.06	1.26	1.33	6	1
1	A	86	TYR	CE2-CZ	5.05	1.45	1.38	9	1
1	A	109	TYR	CG-CD2	5.04	1.45	1.39	4	1
1	A	168	PRO	N-CD	-5.02	1.40	1.47	6	1
2	B	10	G	C5'-C4'	5.02	1.57	1.51	10	1

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
2	B	2	C	N1-C2-O2	19.01	130.30	118.90	1	6
2	B	8	A	C8-N9-C4	-17.65	98.74	105.80	6	5
1	A	88	ARG	NE-CZ-NH1	17.04	128.82	120.30	5	4
2	B	4	C	C2-N3-C4	-16.79	111.51	119.90	2	4
2	B	3	U	O4'-C1'-N1	16.78	121.63	108.20	6	7
2	B	8	A	N9-C4-C5	16.29	112.32	105.80	6	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	8	A	C5-C6-N1	15.43	125.42	117.70	10	6
1	A	68	ARG	NE-CZ-NH1	15.34	127.97	120.30	5	6
2	B	7	A	N1-C6-N6	-14.99	109.61	118.60	9	6
2	B	10	G	C5-C6-O6	14.82	137.49	128.60	3	4
1	A	88	ARG	NE-CZ-NH2	-14.63	112.98	120.30	6	7
1	A	95	ARG	NE-CZ-NH2	-13.96	113.32	120.30	10	3
1	A	95	ARG	NE-CZ-NH1	13.91	127.26	120.30	10	8
1	A	123	TYR	CB-CG-CD1	-13.90	112.66	121.00	7	5
2	B	9	C	N3-C4-C5	13.89	127.46	121.90	9	6
2	B	4	C	N3-C4-C5	13.88	127.45	121.90	2	7
1	A	92	ARG	NE-CZ-NH1	13.80	127.20	120.30	7	4
2	B	4	C	N3-C2-O2	-13.54	112.42	121.90	7	5
2	B	8	A	N1-C6-N6	-13.53	110.48	118.60	9	7
2	B	6	A	N9-C4-C5	13.44	111.17	105.80	6	2
2	B	9	C	N3-C4-N4	-13.41	108.61	118.00	5	4
2	B	7	A	C5-C6-N1	13.35	124.38	117.70	7	5
2	B	2	C	C4-C5-C6	-13.29	110.76	117.40	5	5
1	A	107	ARG	NE-CZ-NH1	13.25	126.93	120.30	10	7
2	B	2	C	N3-C4-C5	13.06	127.12	121.90	5	4
1	A	172	TYR	CB-CG-CD1	-13.03	113.18	121.00	10	6
2	B	2	C	C1'-O4'-C4'	-13.00	99.50	109.90	2	4
2	B	6	A	N1-C6-N6	-12.96	110.83	118.60	8	8
2	B	5	U	O4'-C1'-N1	12.54	118.23	108.20	8	6
2	B	2	C	O4'-C1'-N1	12.41	118.13	108.20	6	7
2	B	10	G	O4'-C1'-N9	12.28	118.02	108.20	10	7
2	B	10	G	N1-C6-O6	-12.27	112.54	119.90	3	2
2	B	10	G	C8-N9-C4	-12.26	101.50	106.40	6	8
2	B	2	C	C5-C4-N4	12.25	128.78	120.20	10	3
2	B	4	C	N1-C2-N3	12.10	127.67	119.20	2	3
2	B	4	C	N3-C4-N4	-12.08	109.54	118.00	6	3
1	A	89	ARG	NE-CZ-NH1	12.05	126.32	120.30	3	8
2	B	8	A	C5-N7-C8	-11.78	98.01	103.90	4	2
2	B	3	U	C2-N3-C4	-11.77	119.94	127.00	3	5
1	A	172	TYR	CB-CG-CD2	11.71	128.02	121.00	10	3
1	A	111	TYR	CB-CG-CD1	-11.70	113.98	121.00	8	7
2	B	6	A	C5-C6-N1	11.70	123.55	117.70	10	6
2	B	8	A	N7-C8-N9	11.63	119.62	113.80	4	3
1	A	88	ARG	NH1-CZ-NH2	-11.61	106.63	119.40	10	3
2	B	5	U	N3-C2-O2	-11.55	114.11	122.20	7	4
2	B	4	C	C5-C4-N4	11.49	128.25	120.20	6	4
1	A	128	ASP	CB-CG-OD1	11.49	128.64	118.30	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	9	C	N3-C2-O2	-11.44	113.89	121.90	8	8
2	B	9	C	N1-C2-O2	11.26	125.66	118.90	4	6
1	A	93	ARG	NE-CZ-NH2	11.19	125.89	120.30	4	8
2	B	3	U	C5-C6-N1	-11.18	117.11	122.70	7	3
2	B	4	C	C6-N1-C2	-11.18	115.83	120.30	7	3
1	A	93	ARG	NE-CZ-NH1	11.14	125.87	120.30	5	6
2	B	10	G	N7-C8-N9	11.09	118.64	113.10	8	4
2	B	10	G	N3-C4-C5	-11.05	123.07	128.60	1	5
1	A	89	ARG	NE-CZ-NH2	-11.04	114.78	120.30	1	6
2	B	10	G	C2-N3-C4	10.91	117.36	111.90	9	2
1	A	149	ARG	NE-CZ-NH1	10.90	125.75	120.30	3	4
1	A	107	ARG	NE-CZ-NH2	-10.85	114.88	120.30	10	5
2	B	7	A	N9-C4-C5	10.83	110.13	105.80	9	3
2	B	2	C	N3-C4-N4	-10.75	110.48	118.00	10	4
2	B	3	U	N1-C2-N3	10.69	121.31	114.90	4	7
2	B	8	A	C5'-C4'-O4'	10.63	121.86	109.10	6	2
2	B	9	C	C3'-C2'-C1'	-10.61	93.02	101.50	5	4
2	B	1	U	N3-C2-O2	-10.59	114.78	122.20	2	6
2	B	4	C	N1-C2-O2	10.56	125.24	118.90	5	4
2	B	2	C	N3-C2-O2	-10.55	114.52	121.90	3	5
2	B	6	A	C6-C5-N7	10.52	139.67	132.30	7	4
2	B	4	C	C5-C6-N1	-10.50	115.75	121.00	4	4
2	B	4	C	O4'-C1'-N1	10.48	116.59	108.20	2	7
1	A	68	ARG	NE-CZ-NH2	10.46	125.53	120.30	10	5
2	B	2	C	C2-N3-C4	-10.37	114.72	119.90	10	4
2	B	10	G	N9-C4-C5	10.35	109.54	105.40	2	6
2	B	1	U	C5-C6-N1	-10.29	117.56	122.70	8	5
2	B	6	A	C4-C5-C6	-10.28	111.86	117.00	10	7
1	A	82	ASP	CB-CG-OD1	10.27	127.55	118.30	4	3
2	B	7	A	C8-N9-C4	-10.26	101.69	105.80	9	3
1	A	149	ARG	NE-CZ-NH2	-10.24	115.18	120.30	1	3
2	B	3	U	N3-C4-O4	-10.23	112.24	119.40	3	4
2	B	6	A	C8-N9-C4	10.13	109.85	105.80	4	4
2	B	2	C	O4'-C4'-C3'	10.13	114.20	106.10	2	2
2	B	3	U	N3-C2-O2	-10.07	115.15	122.20	2	8
2	B	3	U	C3'-C2'-C1'	-10.04	93.47	101.50	5	1
2	B	8	A	O4'-C1'-N9	10.03	116.23	108.20	8	5
2	B	1	U	O5'-P-OP1	-10.00	96.70	105.70	4	2
1	A	128	ASP	CB-CG-OD2	-9.91	109.38	118.30	4	2
2	B	10	G	N1-C2-N3	9.87	129.82	123.90	6	2
2	B	7	A	O4'-C1'-N9	9.86	116.09	108.20	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	2	C	C6-N1-C2	9.59	124.14	120.30	1	3
1	A	109	TYR	CB-CG-CD2	-9.53	115.28	121.00	10	3
1	A	111	TYR	CB-CG-CD2	9.40	126.64	121.00	4	5
2	B	3	U	C5-C4-O4	-9.26	120.35	125.90	8	5
2	B	4	C	C5'-C4'-O4'	9.25	120.20	109.10	7	3
2	B	7	A	C4'-C3'-C2'	-9.24	93.36	102.60	2	2
2	B	7	A	C6-N1-C2	-9.21	113.07	118.60	3	2
2	B	8	A	C3'-C2'-C1'	9.14	108.81	101.50	10	3
2	B	2	C	N1-C2-N3	-9.07	112.85	119.20	1	3
2	B	1	U	C1'-O4'-C4'	-9.05	102.66	109.90	2	3
2	B	9	C	O4'-C1'-C2'	9.02	115.72	107.60	8	1
1	A	72	VAL	CA-CB-CG1	9.01	124.41	110.90	10	2
1	A	89	ARG	NH1-CZ-NH2	-8.99	109.51	119.40	9	1
2	B	7	A	C4-C5-C6	-8.96	112.52	117.00	7	5
2	B	7	A	C5-N7-C8	-8.96	99.42	103.90	7	3
2	B	6	A	C5-C6-N6	8.88	130.80	123.70	6	4
2	B	8	A	C2-N3-C4	8.87	115.03	110.60	10	5
2	B	10	G	C5'-C4'-O4'	-8.75	98.59	109.10	9	2
2	B	5	U	C2-N3-C4	-8.75	121.75	127.00	1	4
2	B	5	U	C3'-C2'-C1'	8.69	108.45	101.50	8	1
2	B	3	U	C4-C5-C6	8.67	124.90	119.70	10	3
2	B	10	G	N3-C4-N9	8.61	131.16	126.00	7	1
1	A	109	TYR	CB-CG-CD1	-8.57	115.86	121.00	1	3
2	B	6	A	C3'-C2'-C1'	8.54	108.33	101.50	4	5
2	B	5	U	N1-C2-O2	-8.48	116.86	122.80	4	3
2	B	7	A	N3-C4-N9	-8.47	120.62	127.40	6	2
2	B	10	G	C5-N7-C8	-8.47	100.06	104.30	8	2
2	B	1	U	C5-C4-O4	8.46	130.98	125.90	5	3
2	B	8	A	C4-C5-N7	-8.43	106.49	110.70	6	3
1	A	174	GLU	OE1-CD-OE2	-8.38	113.24	123.30	8	2
2	B	4	C	C4-C5-C6	-8.32	113.24	117.40	7	3
1	A	93	ARG	NH1-CZ-NH2	-8.30	110.27	119.40	8	3
2	B	6	A	O4'-C1'-N9	8.27	114.81	108.20	4	4
2	B	1	U	N3-C4-O4	-8.25	113.62	119.40	5	1
2	B	9	C	P-O3'-C3'	8.25	129.60	119.70	1	2
2	B	7	A	C3'-C2'-C1'	8.22	108.08	101.50	2	2
1	A	92	ARG	NE-CZ-NH2	-8.21	116.19	120.30	7	4
1	A	108	TRP	NE1-CE2-CD2	-8.19	99.11	107.30	7	3
1	A	50	ALA	N-CA-CB	-8.15	98.68	110.10	5	3
1	A	171	PHE	CB-CG-CD2	-8.15	115.09	120.80	8	2
2	B	5	U	N1-C2-N3	8.09	119.75	114.90	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	6	A	C4-C5-N7	-8.07	106.67	110.70	6	2
2	B	9	C	C6-N1-C2	-8.01	117.09	120.30	8	4
2	B	10	G	N3-C2-N2	-8.01	114.30	119.90	4	4
2	B	9	C	C2-N3-C4	-7.99	115.91	119.90	1	3
2	B	5	U	C5-C6-N1	-7.97	118.71	122.70	5	3
2	B	9	C	C5-C4-N4	7.95	125.76	120.20	5	2
1	A	141	THR	CA-CB-CG2	-7.92	101.31	112.40	3	1
1	A	112	TYR	CB-CG-CD1	-7.92	116.25	121.00	1	2
2	B	7	A	C2-N3-C4	7.91	114.55	110.60	4	5
2	B	2	C	C5-C6-N1	7.87	124.94	121.00	5	1
2	B	7	A	C6-C5-N7	7.87	137.81	132.30	6	3
2	B	6	A	N7-C8-N9	7.85	117.72	113.80	3	2
1	A	132	TRP	CH2-CZ2-CE2	7.83	125.23	117.40	9	2
2	B	1	U	O4'-C1'-N1	7.78	114.42	108.20	1	5
2	B	6	A	C2-N3-C4	7.77	114.48	110.60	8	1
2	B	7	A	N1-C2-N3	-7.75	125.43	129.30	9	3
2	B	8	A	C6-C5-N7	7.72	137.70	132.30	10	1
2	B	9	C	O4'-C1'-N1	7.70	114.36	108.20	4	2
2	B	7	A	N7-C8-N9	7.70	117.65	113.80	7	1
1	A	111	TYR	CG-CD1-CE1	-7.69	115.14	121.30	5	3
1	A	110	PHE	CB-CG-CD1	-7.69	115.42	120.80	2	2
1	A	144	ASP	CB-CG-OD1	-7.67	111.40	118.30	8	1
2	B	10	G	C4-C5-C6	7.66	123.40	118.80	1	2
2	B	3	U	C6-N1-C2	-7.65	116.41	121.00	9	2
1	A	93	ARG	CD-NE-CZ	7.63	134.28	123.60	1	2
2	B	8	A	N3-C4-C5	-7.62	121.47	126.80	6	3
1	A	86	TYR	CB-CG-CD1	-7.61	116.43	121.00	1	2
2	B	1	U	C4-C5-C6	7.58	124.25	119.70	9	4
1	A	115	THR	CA-CB-CG2	7.57	122.99	112.40	4	1
2	B	3	U	O4'-C4'-C3'	7.52	112.11	106.10	10	5
2	B	9	C	C1'-O4'-C4'	-7.51	103.89	109.90	8	4
2	B	10	G	C1'-O4'-C4'	-7.50	103.90	109.90	9	2
1	A	108	TRP	CE2-CD2-CG	7.48	113.28	107.30	10	3
1	A	81	ASP	CB-CG-OD1	7.46	125.01	118.30	10	3
2	B	4	C	C5'-C4'-C3'	-7.41	104.14	116.00	9	4
2	B	1	U	C5'-C4'-C3'	-7.41	104.15	116.00	2	2
1	A	108	TRP	CD1-CG-CD2	-7.35	100.42	106.30	1	4
2	B	1	U	OP1-P-OP2	-7.33	108.61	119.60	6	5
2	B	5	U	C4'-C3'-C2'	-7.30	95.30	102.60	4	2
2	B	4	C	N1-C1'-C2'	-7.29	103.98	112.00	8	2
1	A	87	TYR	CB-CG-CD1	-7.23	116.66	121.00	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	10	G	C6-N1-C2	-7.23	120.76	125.10	6	3
2	B	3	U	N3-C4-C5	7.22	118.93	114.60	3	3
1	A	79	SER	N-CA-CB	-7.17	99.75	110.50	7	1
2	B	10	G	C5-C6-N1	7.15	115.07	111.50	4	3
2	B	5	U	N3-C4-C5	7.13	118.88	114.60	1	2
2	B	6	A	C5-N7-C8	-7.12	100.34	103.90	5	3
2	B	7	A	C1'-O4'-C4'	-7.07	104.25	109.90	10	3
1	A	132	TRP	CD1-NE1-CE2	7.06	115.36	109.00	8	2
2	B	1	U	N1-C2-O2	7.05	127.73	122.80	6	4
1	A	108	TRP	CD1-NE1-CE2	7.00	115.30	109.00	7	2
2	B	7	A	C5'-C4'-O4'	6.99	117.48	109.10	9	1
2	B	6	A	C5'-C4'-C3'	-6.98	104.83	116.00	3	1
1	A	172	TYR	CG-CD2-CE2	6.97	126.88	121.30	1	2
2	B	3	U	N1-C2-O2	6.97	127.68	122.80	2	1
2	B	5	U	C6-N1-C2	-6.96	116.83	121.00	4	2
1	A	63	ASP	CB-CG-OD2	6.95	124.56	118.30	9	5
2	B	7	A	C4-C5-N7	6.93	114.17	110.70	7	2
2	B	9	C	O4'-C4'-C3'	6.90	111.62	106.10	8	3
2	B	3	U	P-O3'-C3'	6.89	127.97	119.70	8	2
1	A	89	ARG	CD-NE-CZ	6.89	133.25	123.60	9	1
2	B	5	U	C5-C4-O4	-6.86	121.79	125.90	1	2
2	B	8	A	C4-C5-C6	-6.83	113.58	117.00	4	4
2	B	6	A	C4'-C3'-C2'	-6.82	95.78	102.60	4	1
2	B	8	A	C4'-C3'-C2'	-6.82	95.78	102.60	3	1
1	A	81	ASP	CB-CG-OD2	6.77	124.39	118.30	9	1
2	B	1	U	C4'-C3'-C2'	-6.76	95.84	102.60	2	1
1	A	109	TYR	CG-CD1-CE1	-6.72	115.92	121.30	1	1
2	B	4	C	P-O3'-C3'	6.70	127.73	119.70	3	2
2	B	10	G	O4'-C4'-C3'	6.70	111.46	106.10	7	3
1	A	144	ASP	CB-CG-OD2	6.69	124.32	118.30	8	1
1	A	132	TRP	NE1-CE2-CD2	-6.68	100.62	107.30	9	2
1	A	112	TYR	CB-CG-CD2	-6.65	117.01	121.00	2	2
1	A	172	TYR	CZ-CE2-CD2	6.63	125.77	119.80	10	1
1	A	112	TYR	CG-CD1-CE1	-6.62	116.00	121.30	1	1
1	A	66	PHE	CB-CG-CD2	6.62	125.44	120.80	6	2
1	A	123	TYR	CB-CG-CD2	6.60	124.96	121.00	3	1
2	B	1	U	N1-C2-N3	6.59	118.85	114.90	1	3
2	B	1	U	C6-N1-C2	6.59	124.95	121.00	8	1
2	B	1	U	O3'-P-O5'	6.58	116.51	104.00	10	1
2	B	10	G	C4-C5-N7	-6.56	108.17	110.80	3	2
2	B	1	U	N3-C4-C5	-6.56	110.66	114.60	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	86	TYR	CZ-CE2-CD2	-6.56	113.90	119.80	8	1
1	A	52	TRP	NE1-CE2-CD2	-6.55	100.75	107.30	3	2
1	A	88	ARG	CD-NE-CZ	6.52	132.73	123.60	8	1
2	B	6	A	O5'-P-OP2	6.50	118.50	110.70	4	1
2	B	6	A	O4'-C4'-C3'	6.50	111.30	106.10	1	2
2	B	8	A	C6-N1-C2	-6.43	114.74	118.60	8	4
1	A	52	TRP	CD2-CE3-CZ3	6.43	127.16	118.80	1	1
1	A	120	GLY	CA-C-O	-6.43	109.03	120.60	10	1
2	B	7	A	C5-C6-N6	6.40	128.82	123.70	6	5
2	B	1	U	C5'-C4'-O4'	6.37	116.75	109.10	1	1
2	B	6	A	C6-N1-C2	-6.37	114.78	118.60	6	1
2	B	8	A	C1'-O4'-C4'	-6.36	104.81	109.90	7	2
1	A	52	TRP	CD1-NE1-CE2	6.35	114.72	109.00	9	3
1	A	68	ARG	NH1-CZ-NH2	-6.33	112.44	119.40	9	2
1	A	161	LEU	CB-CG-CD1	6.32	121.75	111.00	2	1
2	B	2	C	C3'-C2'-C1'	6.31	106.55	101.50	3	1
2	B	5	U	P-O3'-C3'	6.31	127.27	119.70	4	1
2	B	3	U	C2'-C3'-O3'	6.30	123.79	113.70	6	1
1	A	108	TRP	NE1-CE2-CZ2	6.29	137.32	130.40	7	1
2	B	1	U	C2-N3-C4	-6.29	123.23	127.00	5	3
2	B	10	G	C6-C5-N7	-6.25	126.65	130.40	7	3
2	B	4	C	C1'-O4'-C4'	-6.24	104.91	109.90	5	1
2	B	10	G	N1-C2-N2	6.23	121.81	116.20	1	1
1	A	132	TRP	CZ3-CH2-CZ2	-6.22	114.14	121.60	9	1
2	B	6	A	O3'-P-O5'	6.22	115.81	104.00	7	1
2	B	9	C	C5'-C4'-O4'	-6.20	101.67	109.10	4	1
1	A	53	PHE	CB-CG-CD2	6.19	125.14	120.80	4	2
1	A	118	GLU	OE1-CD-OE2	-6.16	115.91	123.30	6	4
2	B	2	C	C5'-C4'-O4'	-6.15	101.72	109.10	9	1
2	B	10	G	N9-C1'-C2'	-6.10	105.29	112.00	9	2
2	B	6	A	N1-C2-N3	-6.09	126.26	129.30	8	2
1	A	72	VAL	CG1-CB-CG2	-6.09	101.16	110.90	3	2
2	B	10	G	O4'-C1'-C2'	6.08	113.07	107.60	4	1
1	A	90	ALA	CB-CA-C	6.07	119.20	110.10	9	1
1	A	123	TYR	CG-CD1-CE1	-6.02	116.49	121.30	7	2
2	B	8	A	C5'-C4'-C3'	-6.01	106.39	116.00	5	1
2	B	5	U	C5'-C4'-O4'	5.97	116.27	109.10	5	1
1	A	132	TRP	NE1-CE2-CZ2	5.95	136.94	130.40	9	2
1	A	104	LEU	CB-CG-CD2	5.92	121.06	111.00	10	2
1	A	62	GLU	OE1-CD-OE2	-5.90	116.22	123.30	10	1
2	B	1	U	C3'-C2'-C1'	5.89	106.22	101.50	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	6	A	N9-C1'-C2'	5.88	121.65	114.00	9	1
1	A	86	TYR	CB-CG-CD2	-5.86	117.48	121.00	4	1
2	B	7	A	N3-C4-C5	-5.86	122.70	126.80	4	1
1	A	103	ASP	CB-CG-OD2	5.83	123.55	118.30	9	3
1	A	86	TYR	CD1-CE1-CZ	5.83	125.05	119.80	7	1
1	A	67	PRO	N-CA-CB	5.81	110.27	103.30	6	1
1	A	82	ASP	CB-CG-OD2	-5.79	113.09	118.30	4	1
1	A	113	LEU	N-CA-CB	-5.79	98.83	110.40	2	1
1	A	162	PRO	N-CD-CG	5.78	111.86	103.20	10	1
2	B	9	C	C4-C5-C6	-5.77	114.51	117.40	10	2
1	A	111	TYR	CG-CD2-CE2	-5.76	116.69	121.30	1	2
1	A	148	THR	CA-CB-CG2	5.76	120.47	112.40	6	1
1	A	122	PRO	N-CA-CB	5.75	110.20	103.30	7	1
1	A	150	ASN	N-CA-CB	-5.75	100.25	110.60	8	1
1	A	106	PRO	N-CA-CB	5.75	110.20	103.30	3	1
1	A	92	ARG	NH1-CZ-NH2	-5.73	113.09	119.40	2	1
2	B	9	C	C2-N1-C1'	5.72	125.10	118.80	5	1
2	B	5	U	C4-C5-C6	5.71	123.13	119.70	6	3
1	A	110	PHE	CB-CG-CD2	5.70	124.79	120.80	2	1
1	A	111	TYR	CD1-CG-CD2	5.68	124.15	117.90	7	2
2	B	5	U	C1'-O4'-C4'	5.68	114.44	109.90	5	1
1	A	57	THR	CA-CB-CG2	5.67	120.33	112.40	10	1
1	A	173	ALA	N-CA-CB	-5.65	102.19	110.10	3	1
1	A	165	THR	CA-CB-CG2	5.64	120.30	112.40	3	1
2	B	4	C	O4'-C1'-C2'	5.61	112.65	107.60	5	1
1	A	134	ALA	N-CA-CB	-5.59	102.27	110.10	9	2
1	A	55	ALA	CB-CA-C	5.58	118.48	110.10	8	1
1	A	70	GLN	O-C-N	-5.57	113.72	123.20	6	1
1	A	92	ARG	CA-CB-CG	5.57	125.66	113.40	9	1
1	A	135	THR	CA-CB-CG2	5.57	120.20	112.40	10	1
1	A	154	ASN	CB-CG-OD1	-5.57	110.46	121.60	5	1
2	B	5	U	O4'-C4'-C3'	-5.57	98.43	104.00	5	2
2	B	7	A	C4-N9-C1'	-5.57	116.28	126.30	6	1
2	B	2	C	C6-N1-C1'	-5.55	114.14	120.80	2	1
1	A	108	TRP	CE2-CD2-CE3	-5.54	112.05	118.70	5	2
1	A	136	GLU	OE1-CD-OE2	-5.53	116.67	123.30	7	1
2	B	6	A	N3-C4-C5	-5.52	122.93	126.80	6	1
1	A	56	LEU	CB-CG-CD1	5.51	120.37	111.00	9	1
2	B	8	A	P-O3'-C3'	5.50	126.30	119.70	5	2
1	A	132	TRP	CD1-CG-CD2	-5.50	101.90	106.30	7	2
2	B	3	U	N1-C1'-C2'	-5.48	105.97	112.00	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	10	G	C3'-C2'-C1'	-5.43	97.16	101.50	9	1
1	A	144	ASP	N-CA-CB	-5.42	100.84	110.60	3	1
1	A	56	LEU	O-C-N	-5.42	114.03	122.70	6	1
1	A	46	PRO	N-CD-CG	5.41	111.32	103.20	3	1
1	A	133	VAL	CA-CB-CG2	5.40	118.99	110.90	9	1
1	A	138	ALA	CB-CA-C	5.39	118.19	110.10	9	1
1	A	65	LYS	CB-CG-CD	-5.39	97.59	111.60	2	1
1	A	108	TRP	CB-CG-CD2	5.37	133.58	126.60	8	1
2	B	8	A	N1-C2-N3	-5.37	126.62	129.30	4	1
1	A	173	ALA	O-C-N	-5.35	114.14	122.70	8	1
2	B	7	A	N9-C1'-C2'	5.34	120.94	114.00	1	1
2	B	2	C	C5'-C4'-C3'	-5.34	107.46	116.00	3	1
1	A	87	TYR	CB-CG-CD2	5.33	124.20	121.00	10	2
1	A	105	SER	N-CA-CB	5.33	118.49	110.50	6	1
2	B	8	A	OP2-P-O3'	5.32	116.90	105.20	1	1
2	B	3	U	C4'-C3'-C2'	-5.29	97.31	102.60	10	1
1	A	52	TRP	CB-CG-CD2	5.28	133.47	126.60	10	1
2	B	1	U	O4'-C4'-C3'	5.28	110.33	106.10	1	1
1	A	109	TYR	CD1-CG-CD2	5.28	123.70	117.90	8	1
1	A	119	ALA	N-CA-CB	-5.27	102.72	110.10	10	1
2	B	9	C	P-O5'-C5'	5.26	129.32	120.90	2	1
1	A	73	PRO	N-CA-CB	5.26	109.61	103.30	3	1
1	A	130	ILE	CA-CB-CG1	5.25	120.98	111.00	10	1
1	A	123	TYR	CD1-CE1-CZ	-5.24	115.08	119.80	3	1
1	A	104	LEU	CB-CG-CD1	-5.21	102.14	111.00	5	1
2	B	4	C	O5'-C5'-C4'	5.21	121.59	111.70	1	1
2	B	7	A	O4'-C4'-C3'	5.18	110.25	106.10	2	1
1	A	68	ARG	CD-NE-CZ	5.17	130.84	123.60	1	1
1	A	60	GLY	O-C-N	-5.17	114.43	122.70	4	1
2	B	5	U	N3-C4-O4	5.15	123.01	119.40	6	1
1	A	57	THR	OG1-CB-CG2	-5.15	98.16	110.00	9	1
1	A	107	ARG	NH1-CZ-NH2	-5.15	113.74	119.40	3	1
2	B	1	U	P-O3'-C3'	5.12	125.84	119.70	8	1
1	A	71	GLY	O-C-N	-5.11	114.52	122.70	7	1
1	A	52	TRP	NE1-CE2-CZ2	5.10	136.01	130.40	1	1
2	B	1	U	O5'-P-OP2	-5.10	101.11	105.70	5	1
2	B	4	C	P-O5'-C5'	5.08	129.03	120.90	7	1
1	A	55	ALA	N-CA-CB	-5.08	102.99	110.10	1	1
1	A	117	PRO	N-CD-CG	5.07	110.81	103.20	2	1
1	A	122	PRO	N-CD-CG	5.07	110.80	103.20	6	1
1	A	142	PRO	N-CD-CG	5.06	110.80	103.20	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	95	ARG	NH1-CZ-NH2	-5.06	113.83	119.40	3	1
2	B	9	C	N1-C1'-C2'	5.06	120.58	114.00	9	1
1	A	163	GLN	C-N-CA	5.04	132.88	122.30	9	1
2	B	9	C	OP1-P-OP2	-5.03	112.05	119.60	1	1
2	B	5	U	OP1-P-OP2	5.03	127.15	119.60	4	1
2	B	9	C	C5'-C4'-C3'	5.03	124.05	116.00	4	1
1	A	135	THR	N-CA-CB	5.03	119.85	110.30	8	1
1	A	112	TYR	CD1-CG-CD2	5.01	123.41	117.90	5	1
1	A	158	VAL	O-C-N	-5.00	114.69	122.70	1	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	6	A	C4',C3'	10

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	6	A	Sidechain	8
2	B	4	C	Sidechain	8
2	B	7	A	Sidechain	7
2	B	2	C	Sidechain	7
2	B	1	U	Sidechain	6
2	B	3	U	Sidechain	5
2	B	5	U	Sidechain	4
2	B	10	G	Sidechain	3
1	A	86	TYR	Sidechain	3
2	B	8	A	Sidechain	3
1	A	87	TYR	Sidechain	3
1	A	93	ARG	Sidechain,Peptide	3
1	A	109	TYR	Sidechain	3
1	A	172	TYR	Sidechain	2
1	A	111	TYR	Sidechain	2
1	A	171	PHE	Sidechain,Peptide	2
2	B	9	C	Sidechain	2
1	A	125	ALA	Peptide,Mainchain	2
1	A	123	TYR	Sidechain	1
1	A	68	ARG	Sidechain	1
1	A	89	ARG	Sidechain	1
1	A	107	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	92	ARG	Sidechain	1
1	A	110	PHE	Mainchain	1
1	A	112	TYR	Sidechain	1
1	A	59	HIS	Sidechain	1
1	A	88	ARG	Sidechain	1
1	A	55	ALA	Peptide	1
1	A	53	PHE	Sidechain	1
1	A	85	GLY	Mainchain	1
1	A	149	ARG	Peptide	1

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	967	939	938	0±0
2	B	210	108	100	0±0
All	All	11770	10470	10426	5

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:PHE:CE2	1:A:87:TYR:CE2	0.51	2.99	8	3
1:A:102:LYS:HE2	2:B:7:A:N3	0.42	2.29	3	1
1:A:110:PHE:CG	1:A:111:TYR:N	0.40	2.89	10	1

6.3 Torsion angles [i](#)

6.3.1 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 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	123/140 (88%)	105±3 (86±2%)	14±3 (11±2%)	4±1 (3±1%)	6	37
All	All	1230/1400 (88%)	1053 (86%)	136 (11%)	41 (3%)	6	37

All 13 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	94	ILE	10
1	A	71	GLY	10
1	A	49	THR	5
1	A	140	ASN	3
1	A	68	ARG	2
1	A	162	PRO	2
1	A	158	VAL	2
1	A	60	GLY	2
1	A	70	GLN	1
1	A	155	ALA	1
1	A	64	LEU	1
1	A	103	ASP	1
1	A	83	GLN	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	99/107 (93%)	98±1 (99±1%)	1±1 (1±1%)	74	96
All	All	990/1070 (93%)	979 (99%)	11 (1%)	74	96

All 8 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	103	ASP	3
1	A	53	PHE	2
1	A	67	PRO	1
1	A	174	GLU	1
1	A	153	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	151	PRO	1
1	A	144	ASP	1
1	A	109	TYR	1

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	9/10 (90%)	5±0 (56±5%)	2±1 (17±7%)	0.18±0.07
All	All	90/100 (90%)	50 (56%)	15 (17%)	0.18

The overall RNA backbone suiteness is 0.18.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	10	G	10
2	B	3	U	10
2	B	7	A	10
2	B	6	A	10
2	B	4	C	8
2	B	9	C	2

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	6	A	10
2	B	9	C	3
2	B	8	A	1
2	B	2	C	1

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 monosaccharides 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 80% 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 [i](#)

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)	21

7.1.2 Chemical shift referencing [i](#)

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 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.02 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.12 ± 0.18	None needed (< 0.5 ppm)
^{15}N	127	-0.53 ± 0.39	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

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. 1343 atoms were assigned a chemical shift out of a possible 1695. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	587/593 (99%)	233/235 (99%)	243/246 (99%)	111/112 (99%)
Sidechain	655/774 (85%)	407/458 (89%)	228/272 (84%)	20/44 (45%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	101/143 (71%)	63/74 (85%)	35/63 (56%)	3/6 (50%)
Overall	1343/1695 (79%)	703/872 (81%)	506/650 (78%)	134/173 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1461 atoms were assigned a chemical shift out of a possible 1823. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	657/663 (99%)	261/263 (99%)	271/274 (99%)	125/126 (99%)
Sidechain	703/832 (84%)	438/493 (89%)	244/291 (84%)	21/48 (44%)
Aromatic	101/143 (71%)	63/74 (85%)	35/63 (56%)	3/6 (50%)
Overall	1461/1823 (80%)	762/935 (81%)	550/697 (79%)	149/191 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	112	TYR	CE1	182.76	124.14 – 111.74	52.3
1	A	87	TYR	CE1	129.73	124.14 – 111.74	9.5
1	A	149	ARG	HB3	-0.55	3.17 – 0.37	-8.3
1	A	89	ARG	HB3	-0.51	3.17 – 0.37	-8.2
1	A	87	TYR	HE2	5.00	7.86 – 5.56	-7.4
1	A	87	TYR	HE1	5.00	7.86 – 5.56	-7.4
1	A	64	LEU	HD11	-1.21	2.16 – -0.64	-7.0
1	A	64	LEU	HD13	-1.21	2.16 – -0.64	-7.0
1	A	64	LEU	HD12	-1.21	2.16 – -0.64	-7.0
1	A	73	PRO	HD3	0.96	5.52 – 1.72	-7.0
1	A	64	LEU	HB3	-0.85	3.34 – -0.26	-6.6
1	A	118	GLU	HB2	0.69	3.08 – 0.98	-6.4
1	A	73	PRO	HG3	-0.10	3.56 – 0.26	-6.1
1	A	71	GLY	HA2	1.75	5.87 – 2.07	-5.8
1	A	64	LEU	HB2	-0.33	3.32 – -0.08	-5.7
1	A	123	TYR	HA	1.62	7.42 – 1.82	-5.3
1	A	64	LEU	HD21	-0.67	2.14 – -0.66	-5.0
1	A	64	LEU	HD22	-0.67	2.14 – -0.66	-5.0
1	A	64	LEU	HD23	-0.67	2.14 – -0.66	-5.0
1	A	87	TYR	HD2	5.43	8.44 – 5.44	-5.0
1	A	87	TYR	HD1	5.43	8.44 – 5.44	-5.0

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.

Random coil index (RCI) for chain A:

