



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 7ACT / pdb_00007act
BMRB ID : 34511
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 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

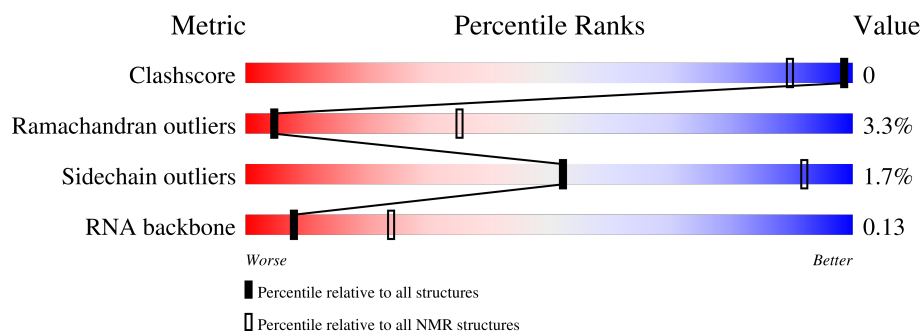
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	 61% 26% 10%
2	B	10	 40% 30% 30%

2 Ensemble composition and analysis

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)	0.78	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 1 clusters and 5 single-model clusters were found.

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

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
1	A	137	Total	C	H	N	O	S	0
			2072	661	1020	192	198	1	

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.

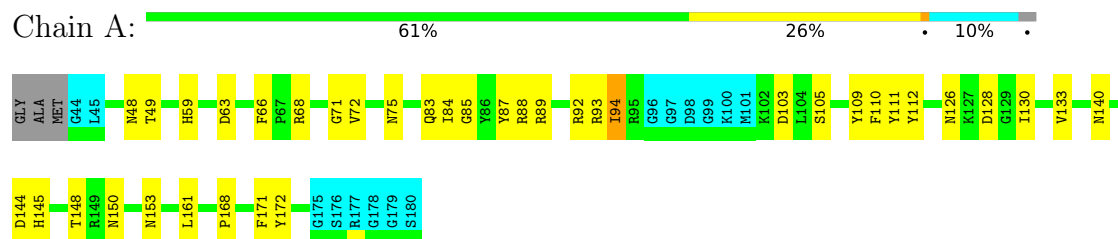
Mol	Chain	Residues	Atoms						Trace
2	B	10	Total	C	H	N	O	P	0
			318	94	108	35	71	10	

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

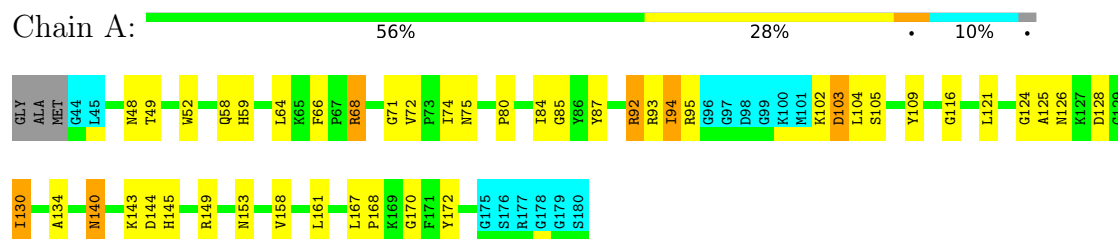


4.2 Scores per residue for each member of the ensemble

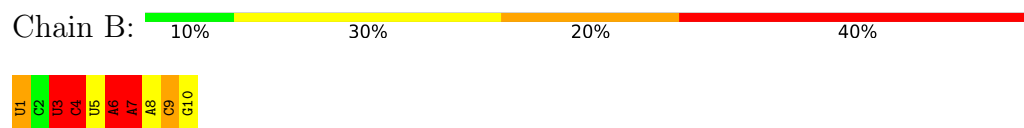
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Nucleoprotein

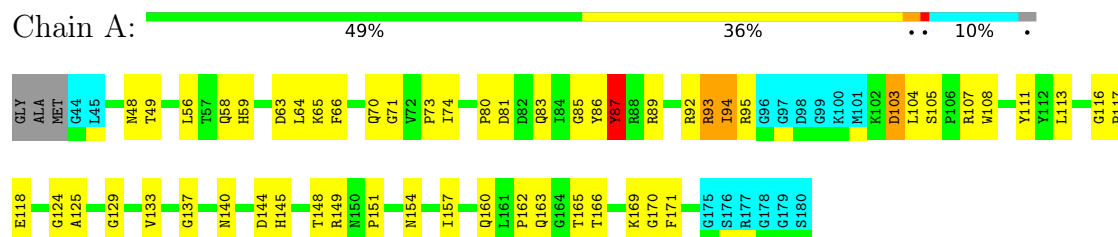


- Molecule 2: ssRNA



4.2.2 Score per residue for model 2

- Molecule 1: Nucleoprotein

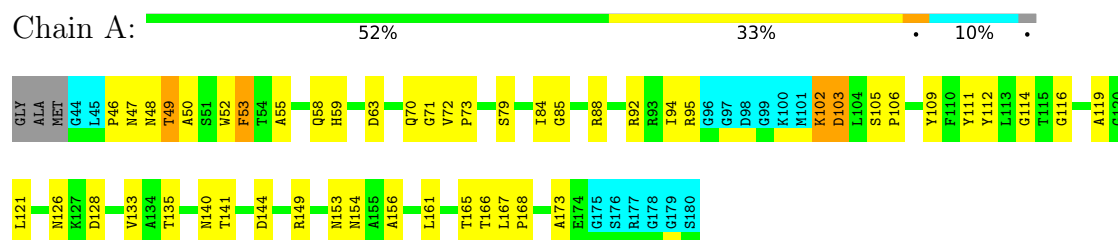


- Molecule 2: ssRNA



4.2.3 Score per residue for model 3

- Molecule 1: Nucleoprotein

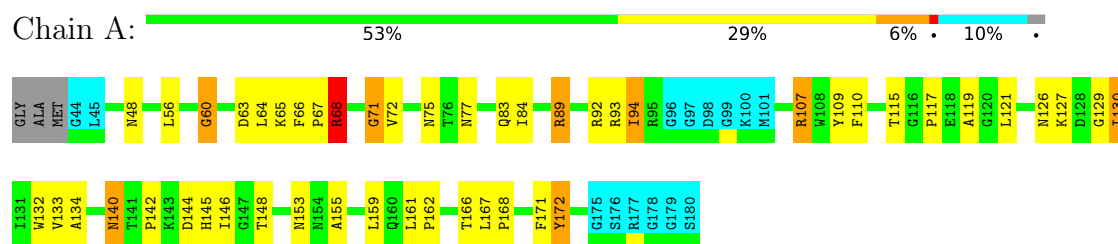


- Molecule 2: ssRNA



4.2.4 Score per residue for model 4

- Molecule 1: Nucleoprotein

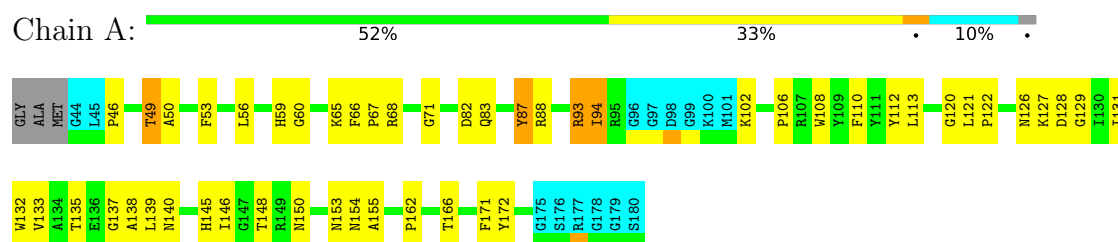


- Molecule 2: ssRNA



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Nucleoprotein

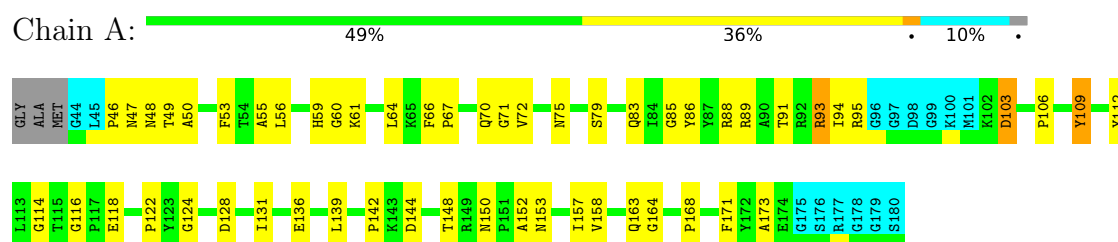


- Molecule 2: ssRNA



4.2.6 Score per residue for model 6

- Molecule 1: Nucleoprotein



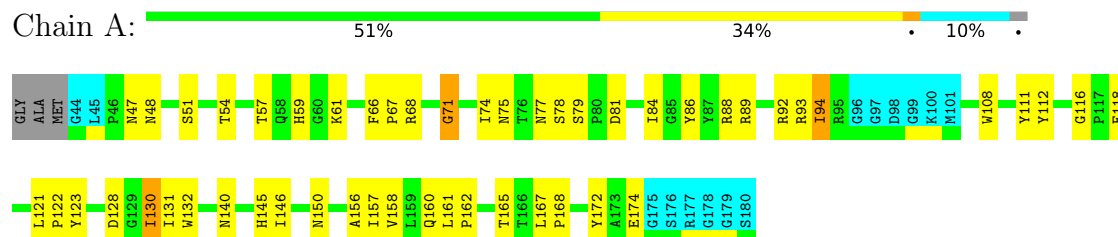
- Molecule 2: ssRNA



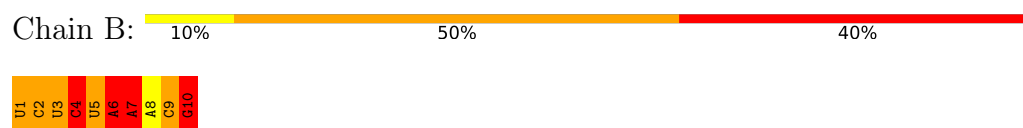


4.2.7 Score per residue for model 7

- Molecule 1: Nucleoprotein

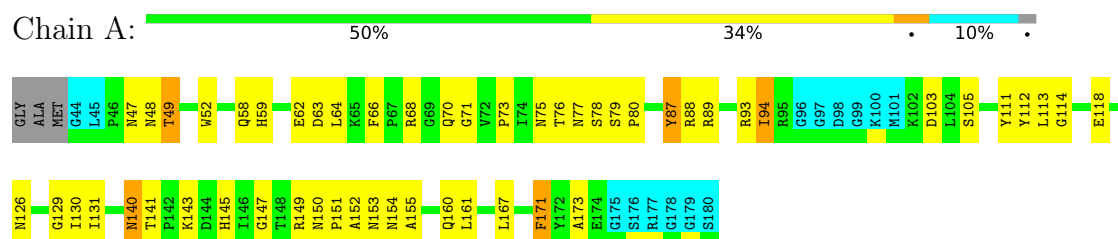


- Molecule 2: ssRNA



4.2.8 Score per residue for model 8

- Molecule 1: Nucleoprotein



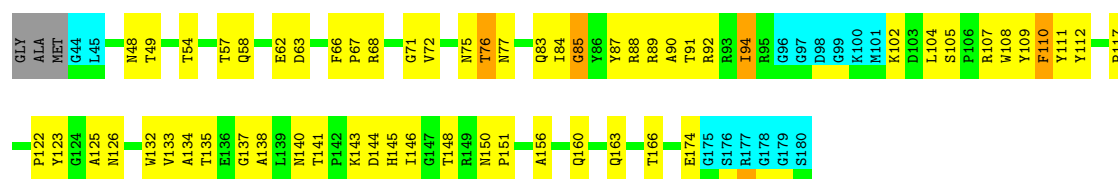
- Molecule 2: ssRNA



4.2.9 Score per residue for model 9

- Molecule 1: Nucleoprotein





- Molecule 2: ssRNA

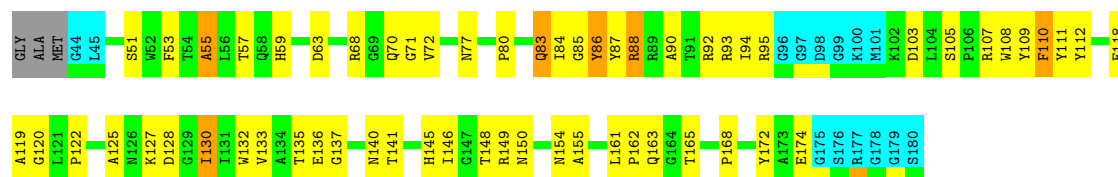
Chain B: 10% 20% 30% 40%



4.2.10 Score per residue for model 10

- Molecule 1: Nucleoprotein

Chain A: 45% 39% 10%



- Molecule 2: ssRNA

Chain B: 10% 20% 40% 30%



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	1637
Number of unparsed shifts	0
Number of shifts with mapping errors	28
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	2.06±0.04	25±3/997 (2.5± 0.3%)	2.32±0.03	48±7/1361 (3.6± 0.5%)
2	B	1.85±0.12	3±1/233 (1.2± 0.4%)	2.08±0.10	13±3/358 (3.7± 0.9%)
All	All	2.02	275/12300 (2.2%)	2.27	617/17190 (3.6%)

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
1	A	118	GLU	N-CA	9.46	1.56	1.46	7	2
1	A	145	HIS	CA-C	9.39	1.65	1.52	2	2
1	A	70	GLN	CA-C	9.18	1.64	1.53	3	1
1	A	49	THR	CA-C	8.98	1.64	1.52	5	3
1	A	72	VAL	CA-C	8.95	1.61	1.53	6	3
1	A	148	THR	CA-C	8.31	1.64	1.52	10	3
1	A	124	GLY	CA-C	8.20	1.62	1.51	1	2
1	A	59	HIS	CB-CG	8.19	1.61	1.50	3	2
1	A	168	PRO	CA-C	7.97	1.62	1.52	4	1
1	A	130	ILE	CA-C	7.93	1.62	1.52	4	2
1	A	95	ARG	N-CA	7.91	1.56	1.45	6	1
2	B	1	U	C5'-C4'	7.91	1.63	1.51	7	1
1	A	67	PRO	N-CD	-7.88	1.36	1.47	4	1
1	A	68	ARG	N-CA	7.75	1.56	1.46	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	9	C	C5'-C4'	7.66	1.62	1.51	4	1
1	A	140	ASN	CA-C	7.62	1.63	1.52	2	4
1	A	94	ILE	N-CA	7.52	1.55	1.46	9	3
1	A	129	GLY	CA-C	7.50	1.62	1.51	2	1
1	A	88	ARG	N-CA	7.43	1.55	1.46	5	3
2	B	1	U	O3'-P	-7.43	1.50	1.61	7	1
2	B	2	C	C3'-O3'	-7.37	1.32	1.43	7	1
1	A	121	LEU	CA-C	7.33	1.61	1.53	4	3
1	A	93	ARG	NE-CZ	7.28	1.41	1.33	1	1
1	A	55	ALA	CA-C	7.23	1.61	1.52	6	2
1	A	106	PRO	CA-C	7.23	1.62	1.52	5	2
1	A	167	LEU	N-CA	7.18	1.55	1.45	7	1
2	B	9	C	C4'-O4'	-7.17	1.35	1.45	5	1
1	A	50	ALA	CA-C	7.14	1.62	1.52	3	1
1	A	154	ASN	CA-C	7.09	1.61	1.52	2	2
1	A	92	ARG	CZ-NH2	-7.08	1.24	1.33	10	1
2	B	6	A	C5'-C4'	7.05	1.61	1.51	2	1
1	A	160	GLN	CA-C	7.04	1.61	1.52	9	1
1	A	162	PRO	CA-C	7.03	1.60	1.52	5	1
2	B	10	G	C2'-O2'	6.84	1.51	1.41	6	1
1	A	108	TRP	N-CA	6.83	1.54	1.46	10	1
1	A	91	THR	N-CA	6.82	1.55	1.46	9	2
1	A	60	GLY	CA-C	6.80	1.61	1.51	5	1
1	A	88	ARG	CZ-NH1	-6.79	1.23	1.32	8	1
1	A	62	GLU	CA-C	6.77	1.61	1.52	9	1
1	A	83	GLN	CA-C	6.73	1.61	1.52	10	3
1	A	73	PRO	CA-C	6.68	1.60	1.52	8	1
1	A	52	TRP	CA-C	6.68	1.61	1.52	8	1
1	A	85	GLY	CA-C	6.67	1.59	1.51	10	4
1	A	166	THR	N-CA	6.66	1.54	1.45	2	1
1	A	48	ASN	CA-C	6.63	1.61	1.52	1	2
1	A	172	TYR	CA-C	6.63	1.60	1.52	7	3
1	A	111	TYR	CA-C	6.61	1.60	1.52	8	1
2	B	6	A	C4'-O4'	-6.61	1.35	1.45	1	1
1	A	66	PHE	CA-C	6.61	1.59	1.52	5	3
1	A	110	PHE	N-CA	6.60	1.53	1.46	4	1
2	B	7	A	P-O5'	6.57	1.69	1.59	7	2
2	B	3	U	O3'-P	-6.55	1.51	1.61	1	1
1	A	105	SER	C-N	6.53	1.41	1.33	8	1
1	A	93	ARG	CZ-NH2	-6.52	1.25	1.33	10	3
1	A	68	ARG	CZ-NH2	-6.50	1.25	1.33	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	TYR	CA-CB	6.47	1.63	1.53	5	1
1	A	134	ALA	N-CA	6.45	1.53	1.45	1	1
1	A	93	ARG	CZ-NH1	-6.42	1.23	1.32	10	1
1	A	144	ASP	CA-C	6.42	1.61	1.52	2	1
1	A	94	ILE	C-O	-6.40	1.16	1.24	2	1
1	A	58	GLN	CA-C	6.39	1.61	1.52	1	2
1	A	133	VAL	N-CA	6.37	1.53	1.46	5	3
1	A	155	ALA	N-CA	6.37	1.54	1.46	4	1
1	A	138	ALA	CA-C	6.37	1.61	1.53	5	1
1	A	107	ARG	CZ-NH2	-6.37	1.25	1.33	10	2
1	A	112	TYR	CA-C	6.34	1.62	1.53	7	3
1	A	111	TYR	N-CA	6.33	1.53	1.46	9	1
1	A	58	GLN	CA-CB	6.33	1.63	1.53	3	1
1	A	66	PHE	C-N	6.32	1.42	1.33	1	1
1	A	133	VAL	CA-C	6.32	1.60	1.52	4	3
1	A	131	ILE	N-CA	6.31	1.54	1.46	8	1
1	A	149	ARG	NE-CZ	6.30	1.40	1.33	1	1
1	A	128	ASP	CA-C	6.29	1.61	1.52	5	2
1	A	79	SER	CA-C	6.26	1.61	1.53	3	3
1	A	109	TYR	CA-C	6.25	1.60	1.52	1	2
1	A	89	ARG	NE-CZ	6.25	1.40	1.33	2	1
1	A	92	ARG	NE-CZ	6.25	1.40	1.33	4	1
1	A	95	ARG	CZ-NH2	-6.24	1.25	1.33	2	3
1	A	150	ASN	N-CA	6.24	1.54	1.46	7	1
1	A	102	LYS	CA-C	6.24	1.60	1.52	1	2
1	A	107	ARG	N-CA	6.19	1.53	1.45	10	1
1	A	87	TYR	CA-C	6.18	1.61	1.52	10	1
1	A	174	GLU	CA-CB	6.17	1.60	1.52	10	1
1	A	130	ILE	N-CA	6.17	1.54	1.46	7	2
2	B	6	A	P-O5'	6.16	1.69	1.59	3	1
1	A	71	GLY	CA-C	6.14	1.60	1.51	4	1
1	A	78	SER	N-CA	6.10	1.54	1.46	7	1
1	A	81	ASP	CA-C	6.09	1.61	1.52	7	1
1	A	89	ARG	CA-C	6.08	1.61	1.53	4	1
1	A	75	ASN	N-CA	6.08	1.54	1.46	8	2
2	B	9	C	O3'-P	-6.07	1.52	1.61	5	1
1	A	167	LEU	C-N	6.06	1.40	1.33	8	1
2	B	10	G	C1'-N9	6.06	1.56	1.47	4	2
1	A	64	LEU	N-CA	6.05	1.53	1.46	4	2
1	A	119	ALA	C-O	-6.04	1.16	1.24	4	2
1	A	153	ASN	CA-C	6.02	1.60	1.52	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	153	ASN	N-CA	6.01	1.53	1.46	4	1
1	A	93	ARG	CA-C	5.98	1.60	1.52	10	1
1	A	66	PHE	CA-CB	5.97	1.60	1.53	6	1
1	A	137	GLY	CA-C	5.97	1.59	1.51	2	3
2	B	6	A	O4'-C1'	5.94	1.50	1.41	6	1
1	A	124	GLY	C-N	5.94	1.42	1.33	6	1
1	A	59	HIS	CA-C	5.92	1.60	1.52	5	2
1	A	159	LEU	CA-C	5.91	1.60	1.52	4	1
1	A	170	GLY	CA-C	5.90	1.60	1.51	1	1
1	A	117	PRO	CA-C	5.88	1.61	1.52	9	1
1	A	165	THR	C-O	-5.87	1.17	1.24	2	1
1	A	120	GLY	CA-C	5.82	1.58	1.52	5	1
1	A	137	GLY	C-N	5.82	1.41	1.33	10	1
1	A	157	ILE	C-O	-5.80	1.18	1.24	2	1
1	A	84	ILE	CA-C	5.77	1.59	1.52	1	2
1	A	65	LYS	C-N	5.77	1.40	1.32	4	1
1	A	92	ARG	CA-C	5.76	1.60	1.53	4	1
1	A	166	THR	CA-C	5.72	1.60	1.52	9	2
1	A	121	LEU	C-N	5.70	1.40	1.33	3	1
1	A	152	ALA	CA-CB	5.69	1.61	1.53	8	1
1	A	152	ALA	CA-C	5.67	1.60	1.53	6	1
1	A	61	LYS	C-O	-5.65	1.18	1.24	7	1
1	A	94	ILE	CA-C	5.64	1.59	1.52	1	2
1	A	88	ARG	NE-CZ	5.64	1.39	1.33	9	1
1	A	85	GLY	C-N	-5.63	1.26	1.33	3	1
1	A	104	LEU	N-CA	5.62	1.53	1.45	1	1
1	A	146	ILE	CA-C	5.61	1.60	1.52	7	3
1	A	150	ASN	C-N	5.59	1.40	1.34	8	2
2	B	7	A	C2'-O2'	5.59	1.50	1.42	9	1
1	A	168	PRO	CA-CB	5.58	1.60	1.53	3	1
2	B	10	G	O4'-C1'	5.57	1.50	1.42	9	1
1	A	161	LEU	N-CA	5.57	1.54	1.45	3	1
1	A	51	SER	N-CA	5.56	1.53	1.46	10	1
1	A	144	ASP	N-CA	5.52	1.53	1.46	6	2
2	B	3	U	C3'-C2'	5.52	1.61	1.52	8	2
1	A	73	PRO	CA-CB	-5.51	1.46	1.53	3	1
1	A	59	HIS	CG-ND1	5.50	1.44	1.38	10	2
1	A	122	PRO	N-CA	-5.50	1.41	1.46	9	1
1	A	93	ARG	CD-NE	5.50	1.53	1.46	5	1
1	A	139	LEU	CA-C	5.48	1.60	1.52	5	2
1	A	112	TYR	N-CA	5.47	1.52	1.45	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	102	LYS	C-O	5.47	1.31	1.24	3	1
1	A	145	HIS	ND1-CE1	-5.46	1.27	1.32	7	1
1	A	92	ARG	N-CA	5.45	1.54	1.46	3	1
1	A	84	ILE	C-O	-5.44	1.17	1.23	3	1
1	A	77	ASN	CA-C	5.44	1.61	1.52	4	1
1	A	46	PRO	N-CA	5.44	1.53	1.47	5	1
1	A	135	THR	N-CA	5.44	1.52	1.45	5	1
1	A	150	ASN	CA-C	5.44	1.59	1.52	7	2
1	A	147	GLY	CA-C	5.41	1.60	1.51	8	1
1	A	87	TYR	C-O	-5.40	1.17	1.23	8	1
1	A	54	THR	CA-C	5.39	1.59	1.52	9	1
1	A	148	THR	N-CA	5.38	1.53	1.46	5	1
2	B	7	A	C2'-C1'	5.38	1.61	1.53	10	1
1	A	142	PRO	CA-C	5.35	1.58	1.52	6	1
1	A	68	ARG	CZ-NH1	-5.35	1.25	1.32	8	1
1	A	89	ARG	N-CA	5.35	1.52	1.46	7	1
2	B	8	A	P-O5'	5.34	1.67	1.59	6	1
1	A	161	LEU	CA-C	5.34	1.59	1.53	7	1
1	A	73	PRO	N-CD	-5.30	1.40	1.47	2	1
1	A	87	TYR	N-CA	-5.28	1.39	1.46	2	1
1	A	147	GLY	C-O	-5.27	1.18	1.24	8	1
1	A	56	LEU	CA-C	5.26	1.59	1.52	2	1
1	A	83	GLN	N-CA	5.25	1.52	1.46	4	1
1	A	128	ASP	N-CA	5.24	1.52	1.46	1	1
1	A	143	LYS	C-N	-5.23	1.27	1.33	1	1
1	A	107	ARG	NE-CZ	5.21	1.38	1.33	2	1
1	A	108	TRP	CA-C	5.20	1.58	1.52	2	1
2	B	1	U	P-O5'	-5.20	1.51	1.59	3	1
1	A	167	LEU	CA-C	5.19	1.59	1.53	3	1
1	A	106	PRO	C-O	5.19	1.30	1.24	6	1
1	A	163	GLN	C-N	5.19	1.40	1.33	6	1
2	B	5	U	P-O5'	-5.19	1.51	1.59	4	1
1	A	143	LYS	CA-CB	5.18	1.60	1.52	1	1
1	A	127	LYS	CA-C	5.18	1.59	1.52	5	1
2	B	4	C	P-O5'	5.17	1.67	1.59	3	1
1	A	49	THR	N-CA	5.17	1.52	1.46	3	1
1	A	102	LYS	N-CA	5.17	1.51	1.46	9	1
1	A	171	PHE	CA-C	5.16	1.59	1.52	5	1
1	A	132	TRP	CA-C	5.16	1.59	1.52	4	1
1	A	105	SER	N-CA	5.15	1.52	1.45	9	1
1	A	131	ILE	CA-C	5.14	1.58	1.52	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	93	ARG	C-O	-5.13	1.17	1.24	6	1
1	A	160	GLN	N-CA	5.12	1.52	1.46	9	1
2	B	9	C	C2'-C1'	-5.12	1.45	1.53	6	1
1	A	79	SER	C-O	-5.11	1.17	1.23	8	1
1	A	174	GLU	N-CA	5.11	1.52	1.46	9	2
1	A	127	LYS	N-CA	5.09	1.52	1.46	10	1
1	A	80	PRO	CA-C	5.08	1.59	1.52	10	1
2	B	6	A	C2'-C1'	-5.08	1.45	1.53	5	1
1	A	104	LEU	C-N	5.08	1.41	1.33	2	1
1	A	155	ALA	CA-C	5.07	1.59	1.53	8	1
1	A	130	ILE	CA-CB	5.06	1.61	1.54	10	1
1	A	129	GLY	N-CA	5.05	1.52	1.44	5	1
1	A	146	ILE	CA-CB	5.04	1.63	1.54	7	1
1	A	118	GLU	CA-C	5.03	1.59	1.52	2	1
1	A	95	ARG	NE-CZ	5.02	1.38	1.33	1	1
1	A	75	ASN	CA-CB	5.02	1.61	1.53	4	1
1	A	142	PRO	N-CA	5.02	1.53	1.47	4	1
2	B	9	C	C4-N4	-5.02	1.24	1.33	10	1
2	B	9	C	C2'-O2'	5.01	1.49	1.41	7	1
1	A	149	ARG	CZ-NH1	-5.01	1.25	1.32	10	1
1	A	89	ARG	C-N	5.01	1.39	1.33	6	1
1	A	119	ALA	CA-C	5.01	1.59	1.52	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
1	A	103	ASP	CA-CB-CG	11.16	123.76	112.60	2	4
1	A	48	ASN	OD1-CG-ND2	-11.14	111.46	122.60	8	5
1	A	160	GLN	OE1-CD-NE2	-10.28	112.32	122.60	2	2
2	B	2	C	C1'-O4'-C4'	-10.20	99.50	109.70	2	2
1	A	140	ASN	OD1-CG-ND2	-10.13	112.47	122.60	8	4
1	A	105	SER	CA-C-N	10.01	130.64	119.93	10	3
1	A	105	SER	C-N-CA	10.01	130.64	119.93	10	3
1	A	161	LEU	CA-C-N	9.81	132.11	119.84	4	2
1	A	161	LEU	C-N-CA	9.81	132.11	119.84	4	2
1	A	88	ARG	NH1-CZ-NH2	-9.75	106.63	119.30	10	3
2	B	3	U	C2'-C3'-O3'	9.53	123.79	109.50	6	3
1	A	153	ASN	N-CA-C	9.50	122.64	111.71	5	2
1	A	72	VAL	CA-C-N	9.46	129.29	120.21	1	4
1	A	72	VAL	C-N-CA	9.46	129.29	120.21	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	GLN	OE1-CD-NE2	-9.29	113.31	122.60	3	4
2	B	7	A	C4'-C3'-C2'	-9.24	93.36	102.60	2	2
1	A	126	ASN	OD1-CG-ND2	-9.23	113.37	122.60	3	3
1	A	53	PHE	CA-CB-CG	9.21	123.01	113.80	6	2
1	A	63	ASP	CA-CB-CG	9.18	121.78	112.60	3	5
1	A	174	GLU	CA-C-N	9.11	130.53	122.43	9	1
1	A	174	GLU	C-N-CA	9.11	130.53	122.43	9	1
1	A	167	LEU	CA-C-N	9.02	129.05	119.76	7	3
1	A	167	LEU	C-N-CA	9.02	129.05	119.76	7	3
2	B	3	U	O4'-C1'-N1	8.95	121.63	108.20	6	2
1	A	140	ASN	CA-CB-CG	8.79	121.39	112.60	5	3
1	A	167	LEU	CA-C-O	-8.71	111.20	120.70	7	1
2	B	9	C	C3'-C2'-C1'	-8.48	93.02	101.50	5	4
1	A	83	GLN	OE1-CD-NE2	-8.48	114.12	122.60	10	3
1	A	149	ARG	CA-C-O	-8.47	113.11	122.01	1	2
2	B	1	U	O3'-P-O5'	8.34	116.51	104.00	10	2
1	A	72	VAL	CA-CB-CG1	8.24	124.41	110.40	10	2
1	A	150	ASN	CA-C-N	8.21	128.91	120.04	8	2
1	A	150	ASN	C-N-CA	8.21	128.91	120.04	8	2
2	B	9	C	O4'-C1'-C2'	8.12	115.72	107.60	8	2
2	B	2	C	O4'-C4'-C3'	8.10	114.20	106.10	2	2
1	A	77	ASN	CA-CB-CG	8.06	120.66	112.60	7	2
2	B	8	A	C5'-C4'-O4'	8.04	121.86	109.80	6	1
2	B	3	U	C3'-C2'-C1'	-8.03	93.47	101.50	5	1
2	B	4	C	C5'-C4'-C3'	-7.91	104.14	116.00	9	5
2	B	1	U	C5'-C4'-C3'	-7.90	104.15	116.00	2	2
2	B	6	A	O3'-P-O5'	7.88	115.81	104.00	7	1
1	A	67	PRO	N-CA-CB	7.82	110.27	103.31	6	1
1	A	128	ASP	CA-CB-CG	7.81	120.41	112.60	10	3
1	A	116	GLY	CA-C-N	7.77	127.43	119.19	7	5
1	A	116	GLY	C-N-CA	7.77	127.43	119.19	7	5
1	A	50	ALA	N-CA-CB	-7.72	98.68	110.42	5	2
2	B	5	U	O4'-C4'-C3'	-7.67	98.43	106.10	5	1
1	A	171	PHE	CA-CB-CG	7.62	121.42	113.80	8	2
2	B	9	C	O4'-C4'-C3'	7.62	111.62	104.00	8	4
1	A	89	ARG	NH1-CZ-NH2	-7.53	109.51	119.30	9	1
1	A	140	ASN	CA-C-N	7.52	130.84	120.39	4	2
1	A	140	ASN	C-N-CA	7.52	130.84	120.39	4	2
2	B	8	A	C3'-C2'-C1'	7.51	108.81	101.30	10	3
1	A	173	ALA	O-C-N	-7.51	114.14	122.92	8	2
2	B	6	A	C5'-C4'-C3'	-7.45	104.83	116.00	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	158	VAL	O-C-N	-7.45	114.69	122.66	1	1
1	A	93	ARG	NE-CZ-NH2	7.44	125.89	119.20	4	3
2	B	5	U	C4'-C3'-O3'	7.42	120.53	109.40	1	1
1	A	83	GLN	CA-C-N	7.41	133.29	121.95	2	2
1	A	83	GLN	C-N-CA	7.41	133.29	121.95	2	2
1	A	75	ASN	CA-C-N	7.36	133.01	120.72	7	1
1	A	75	ASN	C-N-CA	7.36	133.01	120.72	7	1
1	A	115	THR	CA-CB-CG2	7.35	122.99	110.50	4	1
1	A	49	THR	CA-C-N	7.32	131.81	120.75	8	1
1	A	49	THR	C-N-CA	7.32	131.81	120.75	8	1
1	A	88	ARG	NE-CZ-NH1	7.32	128.82	121.50	5	2
2	B	5	U	C4'-C3'-C2'	-7.30	95.30	102.60	4	2
2	B	6	A	O4'-C4'-C3'	7.30	111.30	104.00	1	4
1	A	163	GLN	OE1-CD-NE2	-7.30	115.30	122.60	2	2
2	B	10	G	O4'-C1'-C2'	7.27	113.07	105.80	4	2
1	A	154	ASN	OD1-CG-ND2	-7.26	115.34	122.60	10	2
2	B	1	U	C1'-O4'-C4'	-7.24	102.66	109.90	2	1
1	A	143	LYS	CA-C-N	7.23	130.94	120.38	8	1
1	A	143	LYS	C-N-CA	7.23	130.94	120.38	8	1
1	A	88	ARG	NE-CZ-NH2	7.17	125.65	119.20	10	4
1	A	61	LYS	CA-C-N	7.16	130.98	120.95	6	1
1	A	61	LYS	C-N-CA	7.16	130.98	120.95	6	1
1	A	47	ASN	OD1-CG-ND2	-7.15	115.45	122.60	8	4
1	A	93	ARG	CD-NE-CZ	7.05	134.28	124.40	1	2
1	A	89	ARG	NE-CZ-NH2	7.05	125.54	119.20	9	1
1	A	68	ARG	NE-CZ-NH2	7.04	125.53	119.20	10	1
1	A	65	LYS	CA-C-N	7.03	132.61	122.98	5	1
1	A	65	LYS	C-N-CA	7.03	132.61	122.98	5	1
2	B	6	A	C3'-C2'-C1'	7.03	108.33	101.30	4	4
2	B	10	G	C5'-C4'-O4'	-7.00	98.59	109.10	9	2
1	A	94	ILE	CA-C-N	6.98	133.21	122.24	4	2
1	A	94	ILE	C-N-CA	6.98	133.21	122.24	4	2
1	A	136	GLU	O-C-N	6.96	130.37	122.22	10	2
2	B	5	U	C3'-C2'-C1'	6.95	108.45	101.50	8	1
1	A	93	ARG	NH1-CZ-NH2	-6.95	110.27	119.30	8	2
2	B	4	C	C5'-C4'-O4'	6.94	120.20	109.80	7	2
1	A	145	HIS	CE1-NE2-CD2	-6.93	102.07	109.00	9	1
1	A	112	TYR	O-C-N	-6.88	114.95	122.79	6	1
1	A	113	LEU	N-CA-CB	-6.87	98.83	109.48	2	1
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	7	A	C3'-C2'-C1'	6.78	108.08	101.30	2	2
2	B	1	U	C4'-C3'-C2'	-6.76	95.84	102.60	2	1
1	A	108	TRP	CE2-CD2-CE3	-6.75	112.05	118.80	5	2
2	B	4	C	O5'-C5'-C4'	6.73	121.59	111.50	1	2
1	A	173	ALA	CA-C-O	6.70	128.48	121.31	6	2
1	A	70	GLN	O-C-N	-6.70	113.72	122.77	6	2
1	A	114	GLY	CA-C-O	6.70	126.40	119.10	8	1
2	B	5	U	O4'-C1'-N1	6.69	118.23	108.20	8	1
1	A	102	LYS	CA-C-O	6.67	127.26	119.32	5	1
1	A	166	THR	CA-C-N	6.67	130.80	120.60	3	2
1	A	166	THR	C-N-CA	6.67	130.80	120.60	3	2
1	A	168	PRO	CA-C-O	-6.65	113.85	121.56	6	1
1	A	120	GLY	CA-C-O	-6.63	109.03	120.57	10	1
2	B	2	C	O4'-C1'-N1	6.62	118.13	108.20	6	1
1	A	122	PRO	N-CA-CB	6.62	110.20	103.25	7	1
1	A	162	PRO	CA-C-N	6.60	131.79	122.08	10	1
1	A	162	PRO	C-N-CA	6.60	131.79	122.08	10	1
1	A	52	TRP	CD2-CE3-CZ3	6.58	127.16	118.60	1	1
1	A	61	LYS	CA-C-O	6.58	126.84	118.54	6	1
2	B	9	C	C2'-C3'-O3'	-6.57	103.85	113.70	9	1
1	A	156	ALA	CA-C-O	-6.56	113.97	121.19	3	1
1	A	51	SER	CA-C-O	-6.55	113.58	121.05	7	1
2	B	10	G	O4'-C1'-N9	6.55	118.02	108.20	10	3
1	A	131	ILE	CA-C-N	6.55	130.78	121.42	7	1
1	A	131	ILE	C-N-CA	6.55	130.78	121.42	7	1
1	A	95	ARG	NE-CZ-NH2	-6.53	113.32	119.20	10	1
1	A	110	PHE	N-CA-C	6.53	120.70	110.32	10	1
1	A	89	ARG	CA-C-N	6.51	133.41	121.94	2	1
1	A	89	ARG	C-N-CA	6.51	133.41	121.94	2	1
1	A	103	ASP	CA-C-O	6.51	129.03	121.28	8	1
2	B	10	G	C1'-C2'-O2'	-6.50	102.04	111.80	4	1
1	A	106	PRO	N-CA-CB	6.49	110.20	103.38	3	1
1	A	119	ALA	CA-C-N	6.49	128.46	120.22	3	1
1	A	119	ALA	C-N-CA	6.49	128.46	120.22	3	1
1	A	145	HIS	CA-C-O	-6.49	113.61	120.55	10	1
1	A	129	GLY	CA-C-N	6.48	131.95	122.94	2	4
1	A	129	GLY	C-N-CA	6.48	131.95	122.94	2	4
1	A	68	ARG	NE-CZ-NH1	6.47	127.97	121.50	5	2
1	A	141	THR	N-CA-C	6.46	118.03	109.83	9	1
1	A	88	ARG	N-CA-C	6.45	120.10	108.69	6	1
2	B	6	A	N9-C1'-C2'	6.43	121.65	112.00	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	8	A	C3'-C2'-O2'	6.41	120.32	110.70	7	2
1	A	78	SER	N-CA-C	6.41	119.07	110.35	8	1
2	B	8	A	C5'-C4'-C3'	-6.41	106.39	116.00	5	1
1	A	121	LEU	CA-C-N	6.40	126.58	120.31	3	1
1	A	121	LEU	C-N-CA	6.40	126.58	120.31	3	1
1	A	72	VAL	O-C-N	-6.38	114.05	121.07	10	1
1	A	75	ASN	OD1-CG-ND2	-6.38	116.22	122.60	1	2
1	A	108	TRP	NE1-CE2-CD2	-6.38	99.11	107.40	7	2
1	A	104	LEU	CA-C-N	6.36	129.23	120.39	9	1
1	A	104	LEU	C-N-CA	6.36	129.23	120.39	9	1
1	A	60	GLY	O-C-N	-6.36	114.43	122.70	4	1
1	A	72	VAL	N-CA-C	6.34	115.16	108.95	6	2
1	A	145	HIS	ND1-CE1-NE2	6.33	114.73	108.40	7	3
2	B	1	U	O4'-C4'-C3'	6.33	110.33	104.00	1	1
1	A	89	ARG	CD-NE-CZ	6.32	133.25	124.40	9	1
1	A	168	PRO	N-CA-CB	6.32	108.95	103.27	10	1
1	A	71	GLY	O-C-N	-6.29	114.52	122.70	7	1
1	A	135	THR	CA-CB-OG1	6.27	119.01	109.60	3	1
2	B	9	C	P-O3'-C3'	6.26	129.60	120.20	1	1
1	A	148	THR	CA-C-O	6.26	125.89	118.69	9	1
2	B	7	A	O4'-C4'-C3'	6.25	110.25	104.00	2	2
1	A	163	GLN	CA-C-N	6.24	132.88	120.77	9	1
1	A	163	GLN	C-N-CA	6.24	132.88	120.77	9	1
1	A	130	ILE	CA-CB-CG1	6.22	120.98	110.40	10	1
1	A	56	LEU	O-C-N	-6.22	114.03	122.36	6	2
1	A	118	GLU	CA-C-N	6.20	129.44	120.38	8	2
1	A	118	GLU	C-N-CA	6.20	129.44	120.38	8	2
1	A	126	ASN	CA-CB-CG	6.20	118.80	112.60	5	2
1	A	50	ALA	CA-C-O	6.18	128.08	121.16	6	1
1	A	85	GLY	CA-C-O	6.17	127.83	121.35	6	1
1	A	110	PHE	CA-CB-CG	6.17	119.97	113.80	5	1
1	A	46	PRO	CA-C-O	-6.15	114.17	121.67	5	1
1	A	56	LEU	CA-C-N	6.15	131.49	122.39	5	1
1	A	56	LEU	C-N-CA	6.15	131.49	122.39	5	1
2	B	3	U	O5'-C5'-C4'	6.14	120.91	111.70	10	1
1	A	74	ILE	N-CA-C	6.12	117.48	109.58	7	1
2	B	5	U	O5'-C5'-C4'	-6.11	102.53	111.70	3	2
1	A	144	ASP	CA-C-O	-6.10	113.36	120.20	9	2
1	A	153	ASN	CB-CG-ND2	6.09	125.54	116.40	8	1
1	A	110	PHE	CA-C-N	6.09	132.65	121.94	9	1
1	A	110	PHE	C-N-CA	6.09	132.65	121.94	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	5	U	C2'-C3'-O3'	6.08	118.63	109.50	10	1
1	A	168	PRO	O-C-N	-6.08	115.67	123.03	7	1
1	A	133	VAL	CA-C-O	6.07	127.47	120.67	2	1
1	A	73	PRO	N-CA-CB	6.06	109.61	103.25	3	1
1	A	89	ARG	N-CA-C	6.03	118.11	110.33	2	1
1	A	171	PHE	CA-C-N	6.02	131.01	122.09	4	1
1	A	171	PHE	C-N-CA	6.02	131.01	122.09	4	1
1	A	122	PRO	O-C-N	-6.02	115.48	122.71	5	1
1	A	48	ASN	CA-C-N	6.02	133.04	121.54	8	2
1	A	48	ASN	C-N-CA	6.02	133.04	121.54	8	2
1	A	150	ASN	CA-CB-CG	6.02	118.62	112.60	10	1
2	B	3	U	O4'-C4'-C3'	6.01	112.11	106.10	10	3
2	B	9	C	C1'-O4'-C4'	-6.01	103.89	109.90	8	3
1	A	126	ASN	N-CA-CB	-6.01	103.20	110.53	1	2
1	A	113	LEU	CB-CA-C	6.00	119.27	109.90	5	2
1	A	155	ALA	CA-C-O	-6.00	114.91	121.87	10	1
1	A	61	LYS	CB-CA-C	5.98	117.24	109.28	7	1
1	A	62	GLU	CB-CA-C	5.98	119.65	109.72	9	1
1	A	79	SER	N-CA-CB	-5.97	99.75	110.37	7	1
1	A	114	GLY	CA-C-N	5.96	132.84	122.82	3	1
1	A	114	GLY	C-N-CA	5.96	132.84	122.82	3	1
2	B	7	A	N9-C1'-C2'	5.96	120.94	112.00	1	1
1	A	65	LYS	CB-CG-CD	-5.96	97.59	111.30	2	1
1	A	88	ARG	CD-NE-CZ	5.95	132.73	124.40	8	1
1	A	132	TRP	CH2-CZ2-CE2	5.95	125.23	117.50	9	1
1	A	135	THR	CA-C-N	5.94	128.52	120.38	9	3
1	A	135	THR	C-N-CA	5.94	128.52	120.38	9	3
1	A	146	ILE	O-C-N	5.94	127.87	121.87	5	1
1	A	131	ILE	CA-CB-CG1	5.92	120.46	110.40	6	1
1	A	144	ASP	CA-CB-CG	5.91	118.51	112.60	1	2
1	A	161	LEU	CA-C-O	-5.90	115.29	120.60	7	1
1	A	157	ILE	CA-CB-CG1	5.90	120.43	110.40	7	1
2	B	2	C	O3'-P-O5'	5.90	112.84	104.00	8	1
1	A	57	THR	CA-C-N	5.89	129.73	121.02	7	1
1	A	57	THR	C-N-CA	5.89	129.73	121.02	7	1
1	A	58	GLN	OE1-CD-NE2	-5.88	116.72	122.60	1	2
1	A	145	HIS	CA-CB-CG	5.88	119.68	113.80	9	1
1	A	148	THR	CA-CB-CG2	5.86	120.47	110.50	6	1
1	A	80	PRO	CA-C-N	5.85	128.70	120.28	1	1
1	A	80	PRO	C-N-CA	5.85	128.70	120.28	1	1
1	A	152	ALA	N-CA-CB	-5.84	103.47	111.65	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	HIS	N-CA-C	-5.83	104.93	112.68	6	2
1	A	156	ALA	N-CA-C	5.83	117.81	110.24	9	2
1	A	132	TRP	CE2-CD2-CE3	-5.82	112.98	118.80	5	3
2	B	10	G	O5'-C5'-C4'	-5.82	102.98	111.70	7	1
1	A	84	ILE	CB-CA-C	5.81	120.75	111.80	10	1
1	A	55	ALA	CA-C-O	-5.81	113.97	120.54	6	2
2	B	10	G	N9-C1'-C2'	-5.81	105.29	114.00	9	2
2	B	10	G	C1'-O4'-C4'	-5.80	103.90	109.70	9	1
1	A	77	ASN	CB-CG-ND2	5.80	125.10	116.40	4	1
1	A	57	THR	CA-CB-CG2	5.79	120.33	110.50	10	1
1	A	94	ILE	O-C-N	-5.78	115.34	122.57	5	1
1	A	92	ARG	CA-CB-CG	5.78	125.66	114.10	9	1
1	A	162	PRO	N-CD-CG	5.78	111.86	103.20	10	1
1	A	90	ALA	CA-C-N	5.77	128.48	120.29	10	1
1	A	90	ALA	C-N-CA	5.77	128.48	120.29	10	1
1	A	168	PRO	CA-C-N	5.76	128.58	120.28	1	1
1	A	168	PRO	C-N-CA	5.76	128.58	120.28	1	1
1	A	165	THR	CA-CB-CG2	5.76	120.30	110.50	3	1
1	A	95	ARG	NE-CZ-NH1	5.76	127.26	121.50	10	1
1	A	59	HIS	CB-CG-CD2	-5.74	123.73	131.20	1	1
2	B	9	C	C4'-C3'-O3'	5.74	121.61	113.00	9	1
1	A	63	ASP	O-C-N	-5.73	116.05	122.75	8	1
1	A	121	LEU	CA-C-O	-5.73	114.66	119.76	7	1
2	B	9	C	N1-C1'-C2'	5.72	120.58	112.00	9	1
1	A	135	THR	CA-CB-CG2	5.71	120.20	110.50	10	1
1	A	93	ARG	CA-C-N	5.70	132.23	121.97	10	2
1	A	93	ARG	C-N-CA	5.70	132.23	121.97	10	2
1	A	92	ARG	NE-CZ-NH1	5.70	127.20	121.50	7	1
1	A	72	VAL	N-CA-CB	-5.69	104.79	110.08	6	1
1	A	150	ASN	N-CA-CB	-5.68	100.25	110.37	8	1
1	A	122	PRO	N-CA-C	5.68	119.93	111.41	10	1
1	A	80	PRO	N-CA-CB	5.68	108.96	103.51	2	1
2	B	8	A	C1'-C2'-O2'	-5.68	99.89	108.40	5	1
1	A	75	ASN	CA-C-O	5.67	127.12	120.20	9	1
1	A	161	LEU	N-CA-C	5.67	118.11	110.29	8	1
1	A	77	ASN	OD1-CG-ND2	-5.67	116.93	122.60	9	2
1	A	132	TRP	CZ3-CH2-CZ2	-5.66	114.14	121.50	9	1
2	B	7	A	C1'-O4'-C4'	-5.66	104.25	109.90	10	1
1	A	153	ASN	CA-CB-CG	5.65	118.25	112.60	1	1
1	A	114	GLY	O-C-N	5.65	129.32	122.32	6	1
1	A	68	ARG	CA-C-N	5.63	130.95	120.87	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	ARG	C-N-CA	5.63	130.95	120.87	4	1
2	B	9	C	P-O5'-C5'	5.61	129.32	120.90	2	1
2	B	1	U	C3'-C2'-O2'	5.60	119.10	110.70	7	1
2	B	4	C	O4'-C4'-C3'	5.60	109.60	104.00	5	1
1	A	112	TYR	CA-C-N	5.59	129.05	121.05	9	1
1	A	112	TYR	C-N-CA	5.59	129.05	121.05	9	1
1	A	140	ASN	CB-CG-ND2	5.58	124.77	116.40	7	1
1	A	144	ASP	N-CA-CB	-5.58	100.84	110.32	3	1
1	A	57	THR	OG1-CB-CG2	-5.57	98.16	109.30	9	1
1	A	105	SER	O-C-N	-5.57	115.40	121.53	2	1
1	A	144	ASP	N-CA-C	5.55	117.79	111.02	1	1
1	A	48	ASN	CA-CB-CG	5.55	118.15	112.60	3	2
1	A	79	SER	CA-C-N	5.54	126.77	119.84	3	3
1	A	79	SER	C-N-CA	5.54	126.77	119.84	3	3
1	A	74	ILE	CA-C-O	5.53	127.69	121.11	2	1
1	A	102	LYS	N-CA-CB	-5.52	102.57	110.80	3	1
1	A	128	ASP	CA-C-N	5.52	130.96	121.07	3	1
1	A	128	ASP	C-N-CA	5.52	130.96	121.07	3	1
1	A	105	SER	CA-C-O	5.52	127.27	120.87	1	3
1	A	141	THR	CA-C-N	5.51	125.42	119.85	8	2
1	A	141	THR	C-N-CA	5.51	125.42	119.85	8	2
1	A	141	THR	CA-C-O	-5.51	114.70	120.70	10	1
1	A	92	ARG	CA-C-N	5.50	131.65	121.52	7	2
1	A	92	ARG	C-N-CA	5.50	131.65	121.52	7	2
1	A	165	THR	N-CA-C	5.50	118.15	109.96	10	1
1	A	68	ARG	O-C-N	-5.49	115.28	122.59	1	1
1	A	107	ARG	NE-CZ-NH2	5.48	124.13	119.20	4	1
2	B	10	G	C2'-C3'-O3'	5.48	117.72	109.50	7	1
1	A	134	ALA	N-CA-C	5.47	117.29	109.14	4	1
1	A	130	ILE	O-C-N	5.46	129.18	122.95	1	1
1	A	153	ASN	CA-C-N	5.46	131.99	122.81	4	1
1	A	153	ASN	C-N-CA	5.46	131.99	122.81	4	1
1	A	67	PRO	CA-C-N	5.45	131.12	122.61	5	2
1	A	67	PRO	C-N-CA	5.45	131.12	122.61	5	2
1	A	92	ARG	CB-CA-C	5.44	120.05	112.11	3	1
2	B	7	A	O3'-P-O5'	5.43	112.15	104.00	3	1
1	A	123	TYR	CB-CG-CD1	-5.43	112.66	120.80	7	1
1	A	107	ARG	NE-CZ-NH1	5.43	126.93	121.50	10	1
2	B	4	C	P-O5'-C5'	5.42	129.03	120.90	7	1
2	B	9	C	C5'-C4'-O4'	-5.42	101.67	109.80	4	1
1	A	134	ALA	N-CA-CB	-5.42	102.84	111.62	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	ASN	N-CA-C	5.42	116.77	109.24	9	1
1	A	68	ARG	CD-NE-CZ	-5.42	116.82	124.40	5	1
1	A	46	PRO	N-CD-CG	5.41	111.32	103.20	3	1
1	A	95	ARG	CB-CA-C	-5.41	102.04	110.37	3	1
2	B	9	C	O3'-P-O5'	-5.41	95.89	104.00	3	1
1	A	161	LEU	CD1-CG-CD2	-5.40	98.91	110.80	1	1
1	A	141	THR	CA-CB-CG2	-5.40	101.31	110.50	3	1
2	B	8	A	O5'-C5'-C4'	5.40	119.59	111.50	1	1
1	A	86	TYR	CA-C-O	5.39	127.03	120.99	10	1
1	A	145	HIS	CB-CG-CD2	-5.39	124.19	131.20	10	1
2	B	4	C	O4'-C1'-N1	5.39	116.59	108.50	2	1
1	A	103	ASP	CA-C-N	5.38	129.40	120.94	3	1
1	A	103	ASP	C-N-CA	5.38	129.40	120.94	3	1
1	A	93	ARG	CA-C-O	-5.37	113.31	119.60	7	1
1	A	150	ASN	OD1-CG-ND2	-5.37	117.23	122.60	8	1
1	A	141	THR	CA-CB-OG1	5.37	117.66	109.60	9	1
2	B	9	C	C5'-C4'-C3'	5.37	124.05	116.00	4	1
1	A	60	GLY	CA-C-N	5.36	131.78	121.54	4	2
1	A	60	GLY	C-N-CA	5.36	131.78	121.54	4	2
2	B	10	G	O4'-C4'-C3'	5.36	111.46	106.10	7	1
2	B	3	U	N1-C1'-C2'	-5.35	105.97	114.00	6	1
1	A	154	ASN	CA-C-N	5.35	131.76	121.54	5	1
1	A	154	ASN	C-N-CA	5.35	131.76	121.54	5	1
1	A	84	ILE	O-C-N	-5.35	116.89	123.09	4	1
1	A	126	ASN	CB-CA-C	5.35	118.57	111.14	8	1
2	B	4	C	N1-C1'-C2'	-5.34	103.98	112.00	8	1
1	A	170	GLY	CA-C-O	-5.34	115.00	120.45	2	1
1	A	94	ILE	CA-CB-CG2	5.34	119.58	110.50	8	1
1	A	111	TYR	CA-C-O	-5.34	115.01	120.99	7	1
2	B	6	A	C2'-C3'-O3'	-5.34	105.69	113.70	7	1
1	A	141	THR	O-C-N	-5.34	118.11	121.85	8	1
2	B	8	A	N9-C1'-C2'	5.33	120.00	112.00	4	1
1	A	68	ARG	N-CA-C	5.32	122.12	110.80	1	1
1	A	150	ASN	CB-CA-C	5.31	116.19	110.08	6	1
2	B	3	U	C4'-C3'-O3'	-5.31	101.44	109.40	6	1
1	A	64	LEU	CA-C-O	5.31	128.10	120.51	8	1
1	A	102	LYS	CA-C-N	5.30	131.67	121.54	1	1
1	A	102	LYS	C-N-CA	5.30	131.67	121.54	1	1
1	A	157	ILE	N-CA-C	-5.29	101.90	108.89	6	1
1	A	76	THR	O-C-N	-5.29	115.34	122.43	8	1
1	A	54	THR	O-C-N	-5.29	116.31	122.81	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	125	ALA	N-CA-C	5.29	117.54	110.35	9	1
2	B	3	U	C4'-C3'-C2'	-5.29	97.31	102.60	10	1
1	A	159	LEU	O-C-N	-5.28	116.30	122.96	4	1
1	A	68	ARG	NH1-CZ-NH2	-5.28	112.44	119.30	9	2
1	A	153	ASN	OD1-CG-ND2	-5.27	117.33	122.60	4	1
1	A	59	HIS	ND1-CG-CD2	-5.27	100.83	106.10	7	1
1	A	73	PRO	CA-N-CD	-5.26	104.64	112.00	3	1
1	A	59	HIS	ND1-CE1-NE2	5.25	113.66	108.40	3	1
1	A	173	ALA	N-CA-CB	-5.25	102.19	111.39	3	1
1	A	58	GLN	N-CA-CB	-5.24	102.34	110.04	9	1
1	A	132	TRP	N-CA-C	5.22	117.86	110.50	10	2
1	A	132	TRP	NE1-CE2-CD2	-5.22	100.62	107.40	9	1
1	A	89	ARG	O-C-N	-5.21	116.53	122.68	2	1
1	A	162	PRO	CA-N-CD	-5.21	104.71	112.00	4	1
1	A	86	TYR	N-CA-C	5.21	116.98	109.07	7	1
1	A	148	THR	CA-CB-OG1	-5.20	101.79	109.60	4	1
1	A	81	ASP	CA-CB-CG	5.20	117.80	112.60	2	1
1	A	59	HIS	CB-CG-ND1	5.19	130.49	122.70	1	1
1	A	92	ARG	N-CA-CB	-5.19	104.30	112.13	2	1
1	A	62	GLU	N-CA-CB	-5.19	102.34	109.97	8	1
1	A	59	HIS	CG-CD2-NE2	5.18	112.38	107.20	7	1
2	B	3	U	P-O3'-C3'	5.18	127.97	120.20	8	1
2	B	4	C	C2'-C3'-O3'	-5.18	105.93	113.70	2	1
1	A	117	PRO	CA-C-N	5.18	131.43	121.54	4	1
1	A	117	PRO	C-N-CA	5.18	131.43	121.54	4	1
1	A	64	LEU	O-C-N	-5.18	115.78	122.61	1	1
2	B	10	G	C3'-C2'-O2'	5.17	122.36	114.60	5	1
1	A	154	ASN	CB-CG-OD1	-5.17	110.46	120.80	5	1
1	A	106	PRO	CA-N-CD	-5.17	104.77	112.00	3	1
1	A	143	LYS	CB-CA-C	5.16	117.62	111.22	9	1
2	B	2	C	C5'-C4'-C3'	-5.16	107.46	115.20	3	1
1	A	76	THR	N-CA-C	-5.16	106.25	112.54	9	1
2	B	8	A	O4'-C1'-N9	5.15	116.23	108.50	8	1
1	A	80	PRO	CA-N-CD	-5.15	104.79	112.00	8	1
1	A	151	PRO	N-CA-CB	5.14	108.08	103.20	8	1
1	A	171	PHE	CB-CA-C	5.14	118.22	109.80	5	1
1	A	131	ILE	N-CA-C	5.14	115.49	107.99	7	1
1	A	103	ASP	N-CA-C	5.13	118.80	111.92	6	1
1	A	109	TYR	N-CA-C	5.13	117.19	109.23	9	1
1	A	146	ILE	CA-C-N	5.13	129.77	120.79	9	1
1	A	146	ILE	C-N-CA	5.13	129.77	120.79	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	165	THR	OG1-CB-CG2	-5.13	99.04	109.30	7	1
1	A	154	ASN	N-CA-CB	-5.12	102.50	110.29	8	1
1	A	138	ALA	CB-CA-C	5.12	118.19	109.53	9	1
2	B	7	A	C5'-C4'-O4'	5.12	117.48	109.80	9	1
1	A	125	ALA	CA-C-N	5.12	129.63	122.05	1	1
1	A	125	ALA	C-N-CA	5.12	129.63	122.05	1	1
1	A	52	TRP	NE1-CE2-CD2	-5.11	100.75	107.40	3	1
1	A	160	GLN	CA-C-O	5.10	126.71	120.99	8	1
1	A	156	ALA	CA-C-N	5.10	128.14	120.69	7	1
1	A	156	ALA	C-N-CA	5.10	128.14	120.69	7	1
1	A	169	LYS	CA-C-N	5.10	126.55	120.13	2	1
1	A	169	LYS	C-N-CA	5.10	126.55	120.13	2	1
2	B	3	U	O4'-C1'-C2'	5.09	110.89	105.80	8	1
1	A	82	ASP	CA-C-N	5.09	131.26	121.54	5	1
1	A	82	ASP	C-N-CA	5.09	131.26	121.54	5	1
2	B	8	A	C1'-O4'-C4'	-5.09	104.81	109.90	7	1
1	A	84	ILE	CA-C-N	5.08	127.48	120.72	7	1
1	A	84	ILE	C-N-CA	5.08	127.48	120.72	7	1
1	A	46	PRO	CA-C-N	5.08	130.71	122.07	6	1
1	A	46	PRO	C-N-CA	5.08	130.71	122.07	6	1
1	A	172	TYR	CB-CG-CD1	-5.08	113.18	120.80	10	1
1	A	49	THR	CA-CB-OG1	5.08	117.22	109.60	6	1
1	A	117	PRO	N-CD-CG	5.07	110.81	103.20	2	1
1	A	108	TRP	CE2-CD2-CG	5.07	113.28	107.20	10	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
2	B	7	A	O4'-C1'-N9	5.06	116.09	108.50	7	1
1	A	90	ALA	CB-CA-C	5.06	119.20	111.76	9	1
1	A	90	ALA	N-CA-CB	-5.06	103.31	112.27	10	1
1	A	133	VAL	CA-CB-CG2	5.06	118.99	110.40	9	1
2	B	4	C	O4'-C1'-C2'	5.05	112.65	107.60	5	1
1	A	131	ILE	O-C-N	-5.05	116.31	122.97	7	1
1	A	47	ASN	CB-CG-ND2	5.05	123.97	116.40	8	1
2	B	2	C	C3'-C2'-C1'	5.04	106.55	101.50	3	1
1	A	94	ILE	CA-CB-CG1	5.04	118.98	110.40	4	1
1	A	145	HIS	CB-CG-ND1	5.04	130.26	122.70	1	1
1	A	164	GLY	CA-C-N	5.04	128.48	121.02	6	1
1	A	164	GLY	C-N-CA	5.04	128.48	121.02	6	1
1	A	74	ILE	CA-CB-CG2	5.03	119.05	110.50	1	1
2	B	5	U	C1'-C2'-O2'	5.03	119.34	111.80	6	1
2	B	4	C	P-O3'-C3'	5.02	127.73	120.20	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	113	LEU	CA-C-O	-5.02	115.67	121.19	8	1
1	A	162	PRO	N-CA-CB	5.01	108.51	103.25	4	1
1	A	149	ARG	CA-C-N	5.01	129.28	121.17	2	1
1	A	149	ARG	C-N-CA	5.01	129.28	121.17	2	1
2	B	2	C	O5'-C5'-C4'	-5.01	104.19	111.70	3	1
2	B	10	G	C5'-C4'-C3'	5.00	122.70	115.20	9	1
1	A	93	ARG	CB-CA-C	5.00	118.70	109.99	10	1
1	A	127	LYS	CA-C-N	5.00	127.95	120.90	4	1
1	A	127	LYS	C-N-CA	5.00	127.95	120.90	4	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	6	A	C3',C4'	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	4	C	Sidechain	8
2	B	6	A	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
1	A	87	TYR	Sidechain	3
1	A	86	TYR	Sidechain	3
1	A	93	ARG	Peptide,Sidechain	3
2	B	8	A	Sidechain	3
1	A	109	TYR	Sidechain	3
2	B	10	G	Sidechain	3
1	A	172	TYR	Sidechain	2
1	A	111	TYR	Sidechain	2
1	A	125	ALA	Mainchain,Peptide	2
1	A	171	PHE	Sidechain,Peptide	2
2	B	9	C	Sidechain	2
1	A	92	ARG	Sidechain	1
1	A	112	TYR	Sidechain	1
1	A	149	ARG	Peptide	1
1	A	68	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	89	ARG	Sidechain	1
1	A	107	ARG	Sidechain	1
1	A	53	PHE	Sidechain	1
1	A	59	HIS	Sidechain	1
1	A	85	GLY	Mainchain	1
1	A	110	PHE	Mainchain	1
1	A	123	TYR	Sidechain	1
1	A	55	ALA	Peptide	1
1	A	88	ARG	Sidechain	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%)	5	35
All	All	1230/1400 (88%)	1053 (86%)	136 (11%)	41 (3%)	5	35

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	71	GLY	10
1	A	94	ILE	10
1	A	49	THR	5
1	A	140	ASN	3
1	A	68	ARG	2
1	A	162	PRO	2
1	A	60	GLY	2
1	A	158	VAL	2
1	A	103	ASP	1
1	A	155	ALA	1
1	A	64	LEU	1
1	A	70	GLN	1
1	A	83	GLN	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	99/107 (93%)	97±1 (98±1%)	2±1 (2±1%)	52	92
All	All	990/1070 (93%)	973 (98%)	17 (2%)	52	92

All 10 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	130	ILE	4
1	A	103	ASP	3
1	A	151	PRO	2
1	A	53	PHE	2
1	A	144	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	109	TYR	1
1	A	153	ASN	1
1	A	67	PRO	1
1	A	89	ARG	1
1	A	76	THR	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	9/10 (90%)	5±0 (56±0%)	2±1 (17±7%)	0.27±0.00
All	All	90/100 (90%)	50 (56%)	15 (17%)	0.27

The overall RNA backbone suiteness is 0.13.

All unique RNA backbone outliers are listed below:

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

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	2	C	1
2	B	8	A	1

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% 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	1637
Number of unparsed shifts	0
Number of shifts with mapping errors	28
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	24

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 28 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	GLY	HA2	3.83	0.000	.
1	A	41	GLY	HA3	3.83	0.000	.
1	A	41	GLY	C	179.457	0.003	1
1	A	41	GLY	CA	43.365	0.035	1
1	A	42	ALA	H	8.596	0.002	1
1	A	42	ALA	HA	4.345	0.000	1
1	A	42	ALA	HB1	1.375	0.000	1
1	A	42	ALA	HB2	1.375	0.000	1
1	A	42	ALA	HB3	1.375	0.000	1
1	A	42	ALA	C	177.766	0.006	1
1	A	42	ALA	CA	52.621	0.023	1
1	A	42	ALA	CB	19.383	0.012	1
1	A	42	ALA	N	123.828	0.003	1
1	A	43	MET	H	8.503	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	MET	HA	4.459	0.000	1
1	A	43	MET	HB2	2.086	0.000	.
1	A	43	MET	HB3	2.013	0.000	.
1	A	43	MET	HE1	2.082	0.000	1
1	A	43	MET	HE2	2.082	0.000	1
1	A	43	MET	HE3	2.082	0.000	1
1	A	43	MET	HG2	2.547	0.000	.
1	A	43	MET	HG3	2.614	0.000	.
1	A	43	MET	C	176.61	0.005	1
1	A	43	MET	CA	55.565	0.039	1
1	A	43	MET	CB	32.871	0.027	1
1	A	43	MET	CE	16.929	0.000	1
1	A	43	MET	CG	32.009	0.033	1
1	A	43	MET	N	119.86	0.004	1

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 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.02 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.12 ± 0.08	None needed (< 0.5 ppm)
^{15}N	127	-0.55 ± 0.22	Should be applied

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 82%, i.e. 1501 atoms were assigned a chemical shift out of a possible 1839. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	600/606 (99%)	246/248 (99%)	243/246 (99%)	111/112 (99%)
Sidechain	797/894 (89%)	538/578 (93%)	239/272 (88%)	20/44 (45%)
Aromatic	104/154 (68%)	63/74 (85%)	38/74 (51%)	3/6 (50%)
Sugar	0/110 (0%)	0/60 (0%)	0/50 (0%)	0/0 (—%)
Base	0/75 (0%)	0/45 (0%)	0/19 (0%)	0/11 (0%)
Overall	1501/1839 (82%)	847/1005 (84%)	520/661 (79%)	134/173 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 82%, i.e. 1632 atoms were assigned a chemical shift out of a possible 1980. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	677/683 (99%)	281/283 (99%)	271/274 (99%)	125/126 (99%)
Sidechain	851/958 (89%)	575/619 (93%)	255/291 (88%)	21/48 (44%)
Aromatic	104/154 (68%)	63/74 (85%)	38/74 (51%)	3/6 (50%)
Sugar	0/110 (0%)	0/60 (0%)	0/50 (0%)	0/0 (—%)
Base	0/75 (0%)	0/45 (0%)	0/19 (0%)	0/11 (0%)
Overall	1632/1980 (82%)	919/1081 (85%)	564/708 (80%)	149/191 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

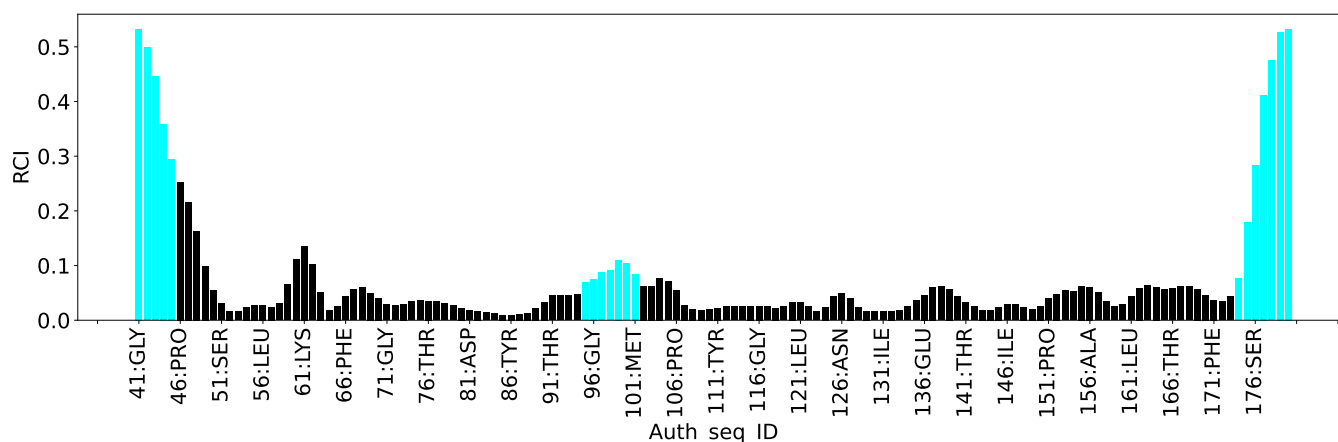
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	112	TYR	CE1	182.76	111.24 – 124.66	48.3
1	A	54	THR	HG1	6.34	0.08 – 2.19	24.6
1	A	165	THR	HG1	5.79	0.08 – 2.19	22.1
1	A	141	THR	HG1	5.78	0.08 – 2.19	22.0
1	A	87	TYR	CE1	129.73	111.24 – 124.66	8.8
1	A	149	ARG	HB3	-0.55	0.43 – 3.11	-8.6
1	A	89	ARG	HB3	-0.51	0.43 – 3.11	-8.5
1	A	87	TYR	HE1	5.00	5.59 – 7.82	-7.6
1	A	87	TYR	HE2	5.00	5.58 – 7.83	-7.5
1	A	64	LEU	HD11	-1.21	-0.61 – 2.12	-7.2
1	A	64	LEU	HD12	-1.21	-0.61 – 2.12	-7.2
1	A	64	LEU	HD13	-1.21	-0.61 – 2.12	-7.2
1	A	73	PRO	HD3	0.96	1.76 – 5.48	-7.1
1	A	64	LEU	HB3	-0.85	-0.26 – 3.31	-6.7
1	A	118	GLU	HB2	0.69	1.00 – 3.05	-6.5
1	A	73	PRO	HG3	-0.10	0.33 – 3.48	-6.3
1	A	71	GLY	HA2	1.75	2.15 – 5.77	-6.1
1	A	64	LEU	HB2	-0.33	-0.07 – 3.30	-5.8
1	A	123	TYR	HA	1.62	1.87 – 7.33	-5.5
1	A	87	TYR	HD1	5.43	5.49 – 8.39	-5.2
1	A	87	TYR	HD2	5.43	5.48 – 8.39	-5.2
1	A	64	LEU	HD21	-0.67	-0.65 – 2.13	-5.1
1	A	64	LEU	HD22	-0.67	-0.65 – 2.13	-5.1
1	A	64	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	7
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	7
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.0
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)	0.3	0.17
0.2-0.5 (Medium)	0.4	0.34
>0.5 (Large)	2.2	2.34

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 ⓘ

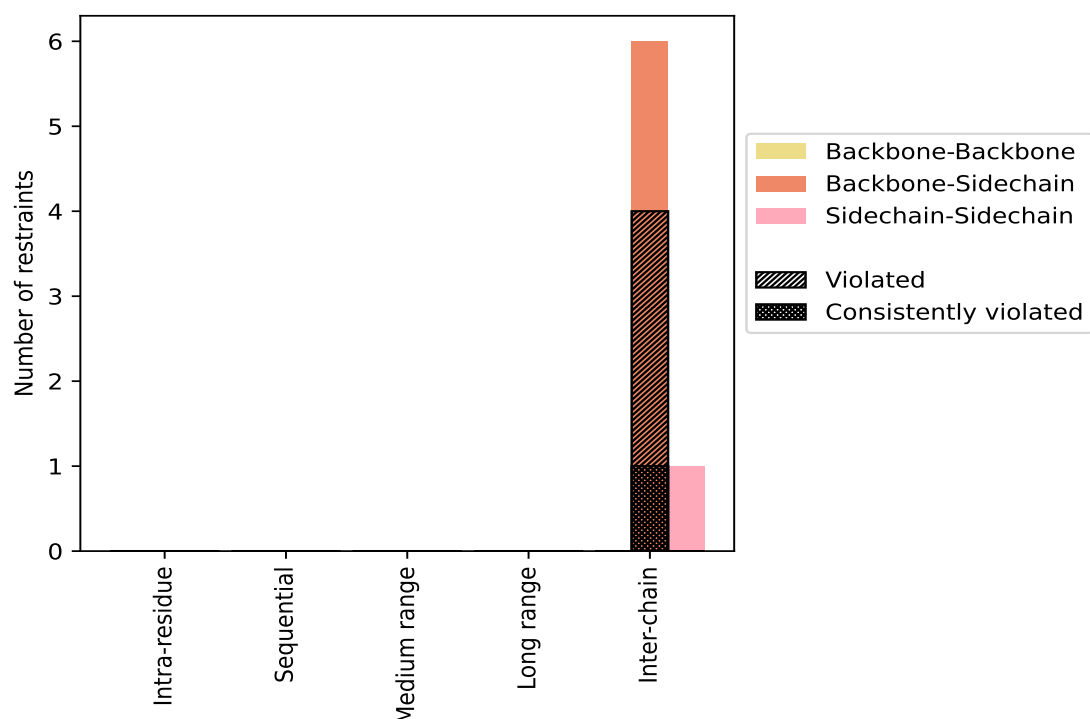
9.1 Summary of distance violations ⓘ

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 \geq 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	7	100.0	4	57.1	57.1	1	14.3	14.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	85.7	4	66.7	57.1	1	16.7	14.3
Sidechain-Sidechain	1	14.3	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	7	100.0	4	57.1	57.1	1	14.3	14.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	85.7	4	66.7	57.1	1	16.7	14.3
Sidechain-Sidechain	1	14.3	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 disulfid bonds are counted in their appropriate category on the x-axis

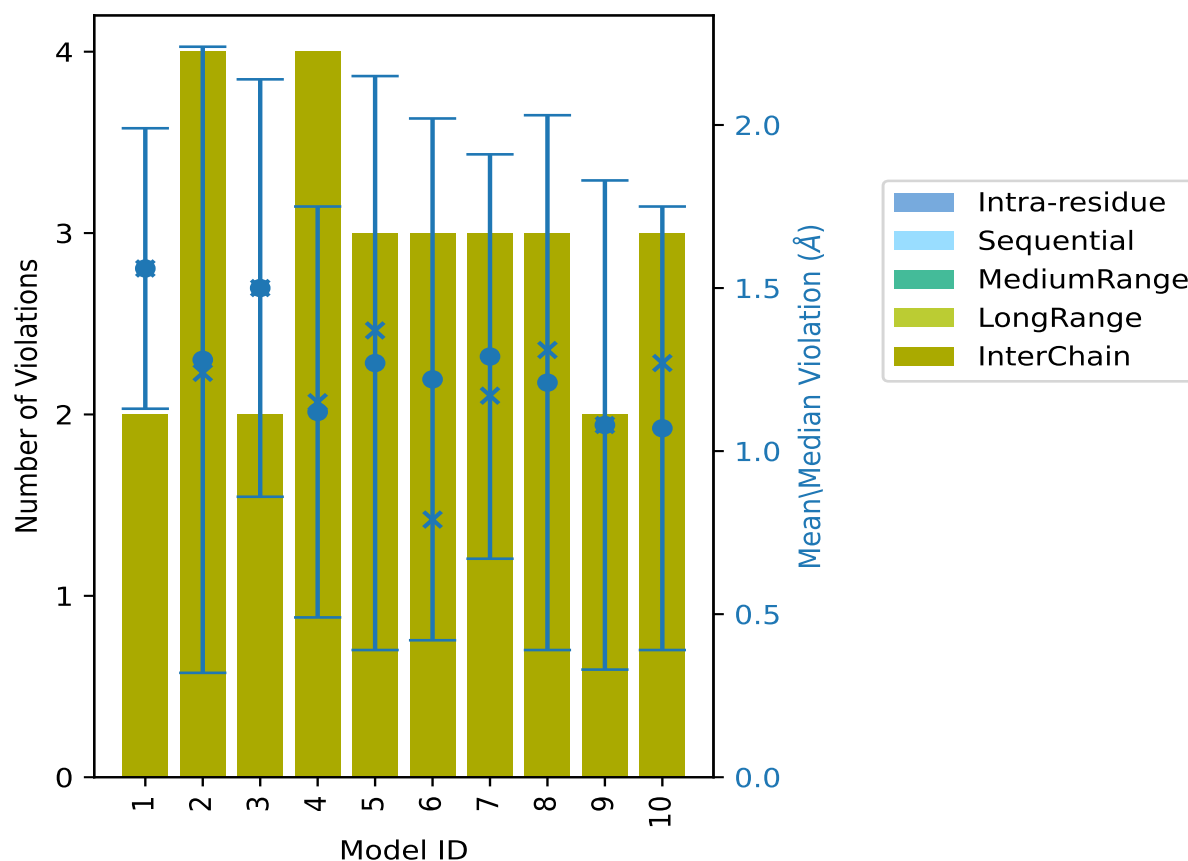
9.2 Distance violation statistics for each model [i](#)

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	2	2	1.56	1.99	0.43	1.56
2	0	0	0	0	4	4	1.28	2.34	0.96	1.24
3	0	0	0	0	2	2	1.5	2.14	0.64	1.5
4	0	0	0	0	4	4	1.12	1.92	0.63	1.15
5	0	0	0	0	3	3	1.27	2.3	0.88	1.37
6	0	0	0	0	3	3	1.22	2.34	0.8	0.79
7	0	0	0	0	3	3	1.29	2.11	0.62	1.17
8	0	0	0	0	3	3	1.21	2.16	0.82	1.31
9	0	0	0	0	2	2	1.08	1.82	0.75	1.08
10	0	0	0	0	3	3	1.07	1.79	0.68	1.27

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 [i](#)



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 [i](#)

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, 3(IR:0, SQ:0, MR:0, LR:0, IC:3) 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	0	0	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

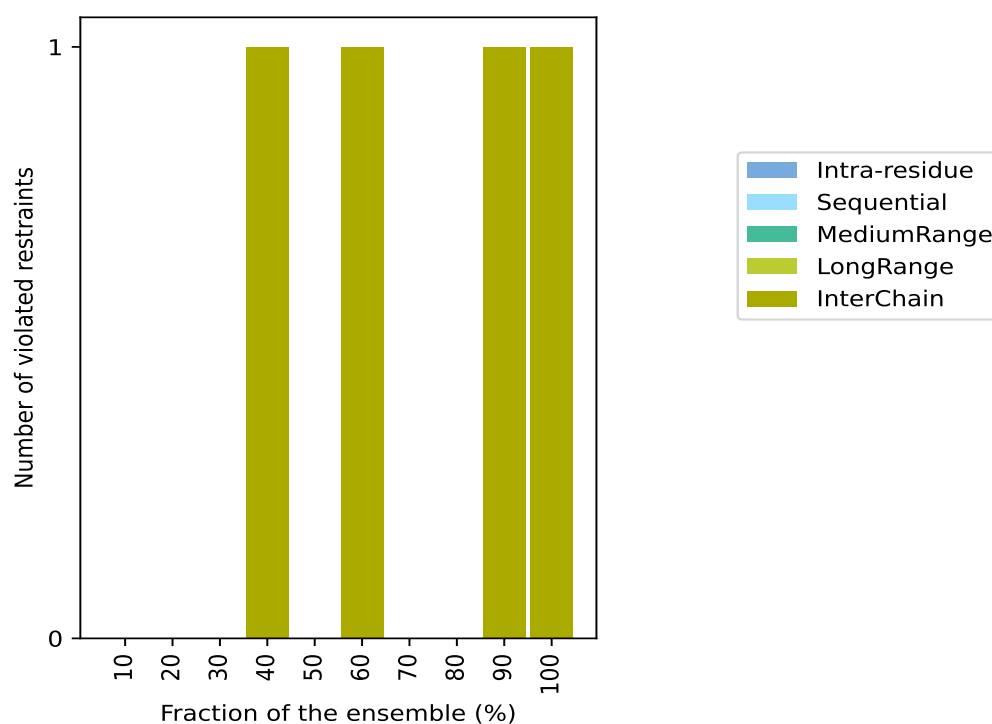
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	1	1	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	1	1	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	1	1	9	90.0
0	0	0	0	1	1	10	100.0

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](#)

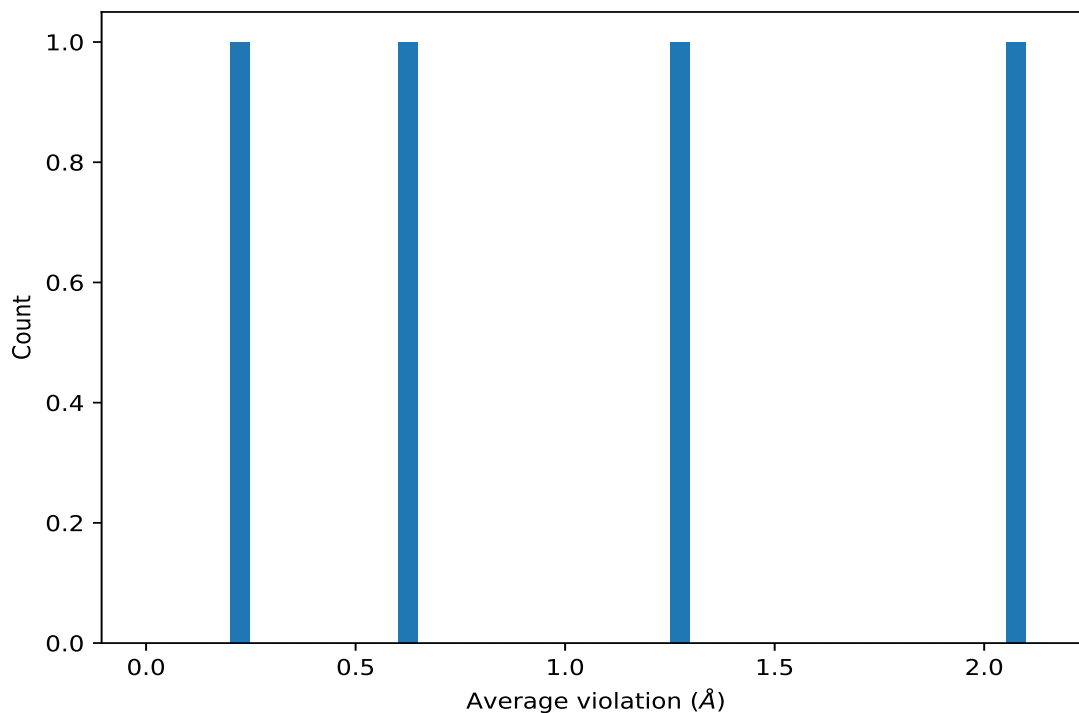


9.4 Most violated distance restraints in the ensemble [i](#)

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 [i](#)

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.

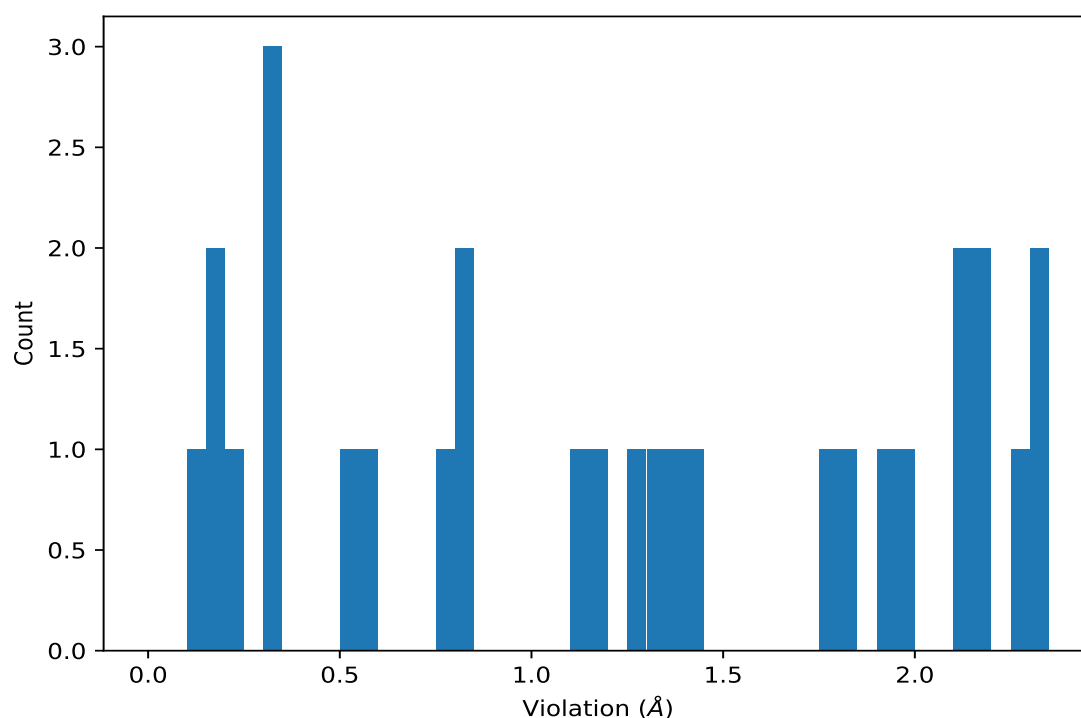
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	10	2.07	0.18	2.12
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	9	1.27	0.47	1.27
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	6	0.22	0.07	0.2
(2,6)	1:107:A:ARG:NE	2:7:B:A:P	4	0.64	0.2	0.7

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)
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	2	2.34
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	6	2.34
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	5	2.3
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	8	2.16
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	2	2.15
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	3	2.14
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	7	2.11
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	1	1.99
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	4	1.92
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	9	1.82
(2,2)	1:88:A:ARG:NH2	2:6:B:A:P	10	1.79
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	4	1.45
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	5	1.37
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	8	1.31
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	10	1.27
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	1	1.14
(2,6)	1:107:A:ARG:NE	2:7:B:A:P	4	0.85
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	3	0.85
(2,6)	1:107:A:ARG:NE	2:7:B:A:P	6	0.79
(2,6)	1:107:A:ARG:NE	2:7:B:A:P	7	0.6
(2,3)	1:61:A:LYS:NZ	2:3:B:U:P	6	0.52
(2,6)	1:107:A:ARG:NE	2:7:B:A:P	2	0.34
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	9	0.33
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	2	0.31
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	4	0.24
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	8	0.17
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	10	0.16
(2,1)	1:177:A:ARG:HH21	2:10:B:G:P	5	0.14

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found