



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 05:09 PM EST

PDB ID : 7B3K
BMRB ID : 34578
Title : Dynamic complex between all-D-enantiomeric peptide D3 with L723P mutant of amyloid precursor protein (APP) 672-726 fragment (amyloid beta 1-55)
Authors : Bocharov, E.V.; Volynsky, P.E.; Okhrimenko, I.S.; Urban, A.S.
Deposited on : 2020-12-01

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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

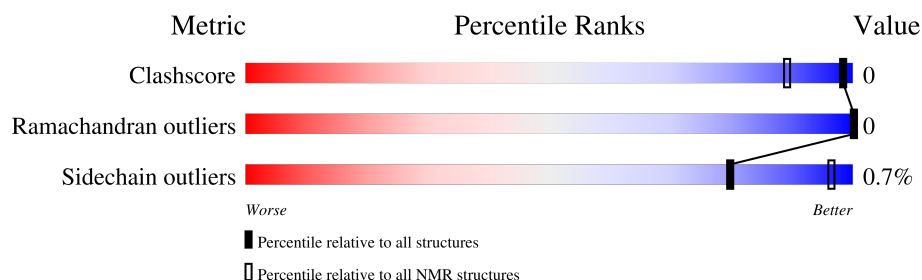
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 97%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	55	<div> <div>40%</div> <div>60%</div> </div>

2 Ensemble composition and analysis

This entry contains 8 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:30-A:51 (22)	0.85	8

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 7, 8
2	1, 2, 3

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1089 atoms, of which 556 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform L-APP677 of Amyloid-beta precursor protein.

Mol	Chain	Residues	Atoms						Trace
1	A	55	Total	C	H	N	O	S	0
			857	272	437	71	75	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	PRO	LEU	engineered mutation	UNP P05067

- Molecule 2 is a protein (with D amino acids) called D3 all D-enantimeric peptide.

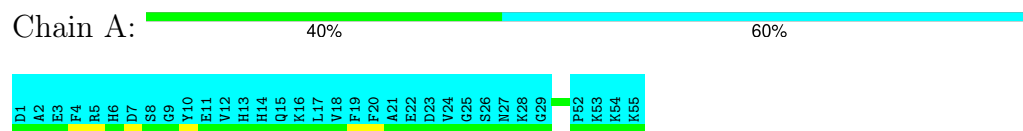
Mol	Chain	Residues	Atoms					Trace
2	B	12	Total	C	H	N	O	0
			232	65	119	32	16	

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: Isoform L-APP677 of Amyloid-beta precursor protein

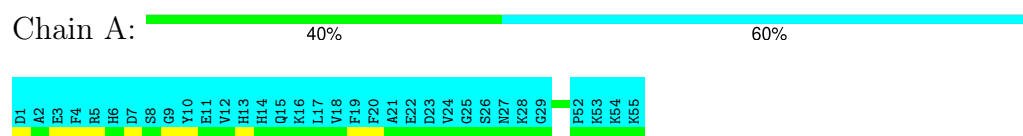


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

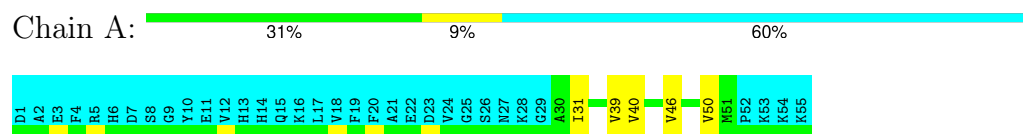
4.2.1 Score per residue for model 1

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



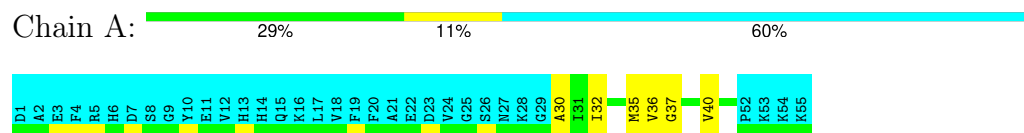
4.2.2 Score per residue for model 2

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



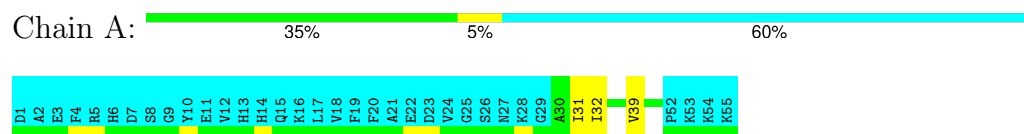
4.2.3 Score per residue for model 3

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



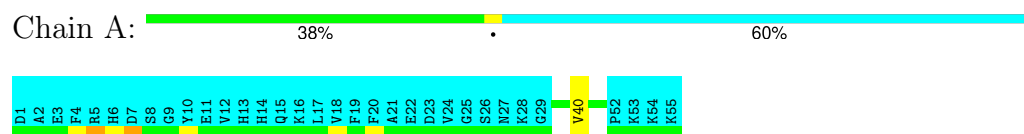
4.2.4 Score per residue for model 4

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



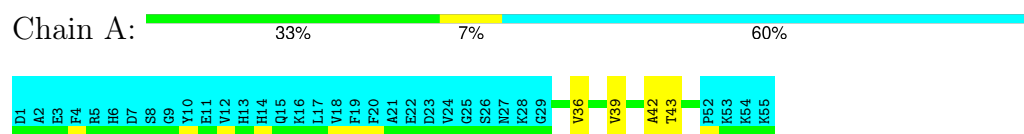
4.2.5 Score per residue for model 5

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



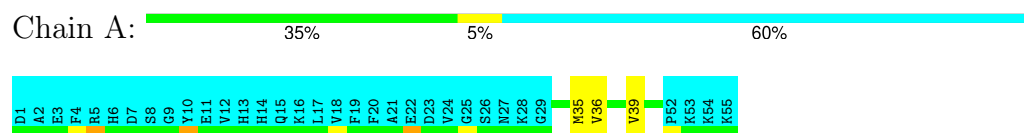
4.2.6 Score per residue for model 6

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



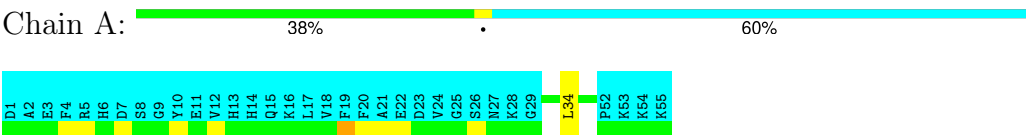
4.2.7 Score per residue for model 7

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Isoform L-APP677 of Amyloid-beta precursor protein



5 Refinement protocol and experimental data overview

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

Of the 8 calculated structures, 8 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
GROMACS	structure calculation	
GROMACS	refinement	

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	645
Number of shifts mapped to atoms	645
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	97%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DSG, 2TL, DLE, DHI, DPR, DAR

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	1.41±0.10	0±0/150 (0.1± 0.2%)	1.78±0.10	2±2/207 (1.2± 0.9%)
2	B	0.00±0.00	-	0.00±0.00	-
All	All	1.41	1/1200 (0.1%)	1.78	20/1656 (1.2%)

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	0.2±0.4
2	B	0.0±0.0	0.1±0.3
All	All	0	3

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	VAL	CA-CB	5.06	1.65	1.54	6	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	50	VAL	CG1-CB-CG2	-9.15	96.26	110.90	2	1
1	A	36	VAL	CG1-CB-CG2	-7.96	98.16	110.90	6	2
1	A	42	ALA	N-CA-CB	-7.59	99.48	110.10	6	1
1	A	40	VAL	CG1-CB-CG2	-6.94	99.79	110.90	2	2
1	A	43	THR	OG1-CB-CG2	-6.45	95.17	110.00	6	1
1	A	39	VAL	CA-CB-CG1	6.21	120.22	110.90	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	VAL	CG1-CB-CG2	-6.21	100.97	110.90	7	1
1	A	35	MET	O-C-N	-6.00	113.10	122.70	3	1
1	A	32	ILE	CA-CB-CG1	5.82	122.07	111.00	3	1
1	A	30	ALA	CB-CA-C	5.57	118.45	110.10	3	1
1	A	37	GLY	C-N-CA	5.54	133.94	122.30	3	1
1	A	40	VAL	CA-CB-CG2	5.52	119.17	110.90	3	1
1	A	46	VAL	CA-CB-CG2	5.36	118.93	110.90	2	1
1	A	32	ILE	CA-CB-CG2	5.24	121.37	110.90	4	1
1	A	36	VAL	CA-CB-CG1	5.20	118.70	110.90	7	1
1	A	36	VAL	CA-CB-CG2	5.20	118.70	110.90	3	1
1	A	34	LEU	CB-CG-CD1	5.16	119.77	111.00	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	31	ILE	Mainchain	2
2	B	101	DAR	Peptide	1

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	150	182	182	0±0
2	B	113	119	114	0±0
All	All	2104	2408	2360	1

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
2:B:106:DLE:HD21	2:B:110:DAR:NH1	0.41	2.30	6	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	22/55 (40%)	20±1 (93±3%)	2±1 (7±3%)	0±0 (0±0%)	100	100
2	B	0	-	-	-	-	-
All	All	176/536 (33%)	164 (93%)	12 (7%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	17/45 (38%)	17±0 (99±2%)	0±0 (1±2%)	80	96
2	B	0	-	-	-	-
All	All	136/360 (38%)	135 (99%)	1 (1%)	80	96

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	35	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics

could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DPR	B	102	2	6,7,8	1.18±0.50	0±0 (6±8%)
2	DLE	B	106	2	5,7,8	0.62±0.20	0±0 (0±0%)
2	DAR	B	105	2	9,10,11	1.32±0.29	1±1 (13±10%)
2	2TL	B	104	2	5,6,7	1.41±0.42	1±1 (20±17%)
2	DAR	B	112	2	10,11,11	1.36±0.24	2±1 (17±9%)
2	DHI	B	107	2	5,10,11	1.04±0.28	0±0 (5±8%)
2	DAR	B	110	2	9,10,11	1.40±0.37	1±1 (15±9%)
2	DSG	B	111	2	6,7,8	1.16±0.20	0±1 (8±11%)
2	DAR	B	101	2	9,10,11	1.38±0.25	1±1 (15±7%)
2	2TL	B	108	2	5,6,7	1.11±0.29	1±1 (12±13%)
2	DHI	B	109	2	5,10,11	1.10±0.32	0±0 (5±8%)
2	DAR	B	103	2	9,10,11	1.33±0.21	1±0 (11±5%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DPR	B	102	2	7,8,10	1.84±0.58	2±1 (21±10%)
2	DLE	B	106	2	6,8,10	1.63±0.37	1±1 (18±9%)
2	DAR	B	105	2	5,11,13	1.77±0.41	1±1 (25±13%)
2	2TL	B	104	2	5,7,9	1.73±0.57	1±1 (22±21%)
2	DAR	B	112	2	9,13,13	1.58±0.48	2±1 (19±14%)
2	DHI	B	107	2	3,12,14	1.23±0.57	0±1 (12±23%)
2	DAR	B	110	2	5,11,13	1.41±0.41	1±1 (17±15%)
2	DSG	B	111	2	4,8,10	1.76±0.30	1±1 (31±16%)
2	DAR	B	101	2	5,11,13	1.95±0.62	2±1 (30±17%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	2TL	B	108	2	5,7,9	1.56±0.41	1±1 (25±21%)
2	DHI	B	109	2	3,12,14	1.67±0.70	1±1 (25±27%)
2	DAR	B	103	2	5,11,13	1.90±0.68	1±1 (25±16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAR	B	112	2	-	0±0,11,11,11	-
2	DHI	B	109	2	-	0±0,5,6,8	0±0,1,1,1
2	DAR	B	101	2	-	0±0,8,9,11	-
2	DPR	B	102	2	-	0±0,0,9,11	0±0,1,1,1
2	DSG	B	111	2	-	0±0,5,6,8	-
2	DAR	B	103	2	-	0±0,8,9,11	-
2	DAR	B	105	2	-	0±0,8,9,11	-
2	DAR	B	110	2	-	0±0,8,9,11	-
2	2TL	B	108	2	-	0±0,5,6,8	-
2	DHI	B	107	2	-	0±0,5,6,8	0±0,1,1,1
2	2TL	B	104	2	-	0±0,5,6,8	-
2	DLE	B	106	2	-	0±0,5,6,8	-

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	110	DAR	CB-CA	5.02	1.61	1.53	4	5
2	B	101	DAR	CB-CA	4.59	1.60	1.53	1	5
2	B	103	DAR	CB-CA	4.28	1.60	1.53	8	1
2	B	102	DPR	CA-N	3.93	1.41	1.48	8	2
2	B	105	DAR	CB-CA	3.69	1.59	1.53	2	4
2	B	104	2TL	OG1-CB	3.64	1.52	1.43	4	2
2	B	101	DAR	CD-NE	3.53	1.54	1.46	3	2
2	B	102	DPR	CD-N	3.44	1.37	1.49	6	1
2	B	112	DAR	CZ-NE	3.41	1.26	1.33	5	1
2	B	112	DAR	OXT-C	3.26	1.20	1.30	7	3
2	B	101	DAR	CZ-NE	3.18	1.27	1.33	4	1
2	B	105	DAR	CZ-NE	3.15	1.27	1.33	4	2
2	B	103	DAR	CD-NE	3.00	1.52	1.46	7	3
2	B	112	DAR	CB-CA	2.97	1.59	1.53	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	109	DHI	CB-CA	2.92	1.59	1.53	7	1
2	B	105	DAR	CA-N	2.79	1.55	1.48	2	2
2	B	108	2TL	CA-N	2.78	1.55	1.47	8	1
2	B	103	DAR	CZ-NE	2.63	1.28	1.33	3	2
2	B	104	2TL	CA-N	2.58	1.55	1.47	2	2
2	B	110	DAR	CD-NE	2.55	1.40	1.46	1	1
2	B	110	DAR	CZ-NE	2.47	1.28	1.33	7	3
2	B	107	DHI	CB-CA	2.45	1.58	1.53	5	1
2	B	112	DAR	CG-CD	2.45	1.61	1.51	3	2
2	B	108	2TL	OG1-CB	2.39	1.36	1.43	3	2
2	B	103	DAR	CA-N	2.39	1.54	1.48	2	1
2	B	101	DAR	CG-CB	2.36	1.62	1.52	1	1
2	B	112	DAR	CG-CB	2.33	1.61	1.52	7	2
2	B	101	DAR	O-C	2.29	1.28	1.20	4	1
2	B	104	2TL	O-C	2.28	1.28	1.20	6	1
2	B	108	2TL	CB-CA	2.27	1.60	1.53	6	1
2	B	111	DSG	CB-CA	2.27	1.58	1.53	4	2
2	B	104	2TL	CG2-CB	2.25	1.58	1.51	5	2
2	B	109	DHI	CD2-NE2	2.22	1.42	1.35	6	1
2	B	110	DAR	O-C	2.21	1.28	1.20	6	2
2	B	111	DSG	CB-CG	2.16	1.57	1.51	6	1
2	B	107	DHI	CB-CG	2.15	1.57	1.51	4	1
2	B	112	DAR	CZ-NH1	2.13	1.26	1.34	2	2
2	B	105	DAR	CD-NE	2.11	1.41	1.46	7	1
2	B	108	2TL	CG2-CB	2.11	1.45	1.51	2	1
2	B	101	DAR	CA-N	2.11	1.53	1.48	8	1
2	B	103	DAR	CZ-NH1	2.11	1.26	1.34	1	1
2	B	112	DAR	CZ-NH2	2.09	1.25	1.32	7	1
2	B	104	2TL	CB-CA	2.05	1.47	1.53	5	1
2	B	105	DAR	CZ-NH1	2.02	1.26	1.34	2	1
2	B	111	DSG	O-C	2.01	1.27	1.20	2	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	102	DPR	CB-CA-C	6.45	103.81	112.66	1	4
2	B	103	DAR	NH1-CZ-NE	5.24	131.17	119.27	8	5
2	B	106	DLE	CB-CA-C	4.93	118.58	110.99	8	5
2	B	101	DAR	NE-CZ-NH2	4.77	112.49	120.67	6	5
2	B	112	DAR	NH1-CZ-NE	4.66	129.86	119.27	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	101	DAR	CB-CG-CD	4.62	125.41	112.07	7	2
2	B	105	DAR	NH1-CZ-NE	4.50	129.48	119.27	3	3
2	B	104	2TL	O-C-CA	4.39	113.47	124.77	2	2
2	B	102	DPR	O-C-CA	4.36	113.55	124.77	3	7
2	B	105	DAR	NE-CZ-NH2	4.33	128.11	120.67	7	3
2	B	104	2TL	OG1-CB-CA	4.07	117.61	109.01	3	3
2	B	103	DAR	NE-CZ-NH2	4.05	113.72	120.67	8	1
2	B	101	DAR	NH1-CZ-NE	3.98	128.32	119.27	4	3
2	B	112	DAR	CB-CA-C	3.98	120.98	110.45	5	3
2	B	104	2TL	CG2-CB-CA	3.83	120.86	112.16	4	3
2	B	112	DAR	NE-CZ-NH2	3.83	114.10	120.67	6	2
2	B	103	DAR	NH1-CZ-NH2	3.82	109.19	120.07	5	3
2	B	109	DHI	CD2-NE2-CE1	3.80	111.73	105.72	7	4
2	B	106	DLE	CB-CA-N	3.79	102.19	110.48	2	3
2	B	103	DAR	CB-CG-CD	3.64	122.57	112.07	3	1
2	B	105	DAR	NH1-CZ-NH2	3.61	109.80	120.07	4	3
2	B	108	2TL	OG1-CB-CG2	3.47	99.30	109.68	7	3
2	B	108	2TL	CG2-CB-CA	3.45	120.00	112.16	8	3
2	B	111	DSG	CA-CB-CG	3.42	119.08	112.21	4	5
2	B	109	DHI	CB-CG-CD2	3.41	121.65	127.75	1	1
2	B	101	DAR	CG-CD-NE	3.34	121.58	112.20	6	2
2	B	111	DSG	CB-CG-ND2	3.33	124.16	116.19	2	2
2	B	111	DSG	OD1-CG-CB	3.32	127.81	120.87	6	1
2	B	110	DAR	NE-CZ-NH2	3.21	126.18	120.67	1	4
2	B	107	DHI	CD2-NE2-CE1	3.20	110.78	105.72	2	2
2	B	105	DAR	CB-CG-CD	3.16	121.18	112.07	1	1
2	B	112	DAR	OXT-C-O	3.15	131.22	124.08	5	2
2	B	112	DAR	CB-CA-N	3.03	102.23	110.12	3	1
2	B	104	2TL	OG1-CB-CG2	2.78	101.37	109.68	4	1
2	B	110	DAR	NH1-CZ-NE	2.76	125.54	119.27	4	1
2	B	110	DAR	NH1-CZ-NH2	2.64	112.55	120.07	8	2
2	B	111	DSG	OD1-CG-ND2	2.59	115.61	122.53	2	2
2	B	108	2TL	O-C-CA	2.55	118.21	124.77	2	2
2	B	108	2TL	OG1-CB-CA	2.42	114.13	109.01	6	2
2	B	109	DHI	CG-CD2-NE2	2.36	104.47	108.81	5	1
2	B	112	DAR	CG-CB-CA	2.30	120.64	113.22	4	1
2	B	107	DHI	CG-CD2-NE2	2.21	104.76	108.81	2	1
2	B	112	DAR	NH1-CZ-NH2	2.19	113.83	120.07	2	1
2	B	112	DAR	CB-CG-CD	2.17	118.34	112.07	2	2
2	B	102	DPR	CD-N-CA	2.16	112.70	107.21	5	1
2	B	112	DAR	CG-CD-NE	2.05	106.46	112.20	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	106	DLE	CD1-CG-CB	2.02	103.83	111.08	4	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 97% for the well-defined parts and 86% 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	645
Number of shifts mapped to atoms	645
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

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
$^{13}\text{C}_\alpha$	54	1.67 ± 0.23	Should be checked
$^{13}\text{C}_\beta$	48	2.86 ± 0.06	Should be checked
$^{13}\text{C}'$	52	2.37 ± 0.11	Should be applied
^{15}N	55	1.13 ± 0.21	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 97%, i.e. 295 atoms were assigned a chemical shift out of a possible 304. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	113/113 (100%)	47/47 (100%)	44/44 (100%)	22/22 (100%)
Sidechain	182/191 (95%)	127/133 (95%)	55/58 (95%)	0/0 (—%)

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	Total	¹ H	¹³ C	¹⁵ N
Overall	295/304 (97%)	174/180 (97%)	99/102 (97%)	22/22 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 643 atoms were assigned a chemical shift out of a possible 750. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	273/279 (98%)	113/115 (98%)	106/110 (96%)	54/54 (100%)
Sidechain	370/411 (90%)	254/272 (93%)	116/129 (90%)	0/10 (0%)
Aromatic	0/60 (0%)	0/31 (0%)	0/26 (0%)	0/3 (0%)
Overall	643/750 (86%)	367/418 (88%)	222/265 (84%)	54/67 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

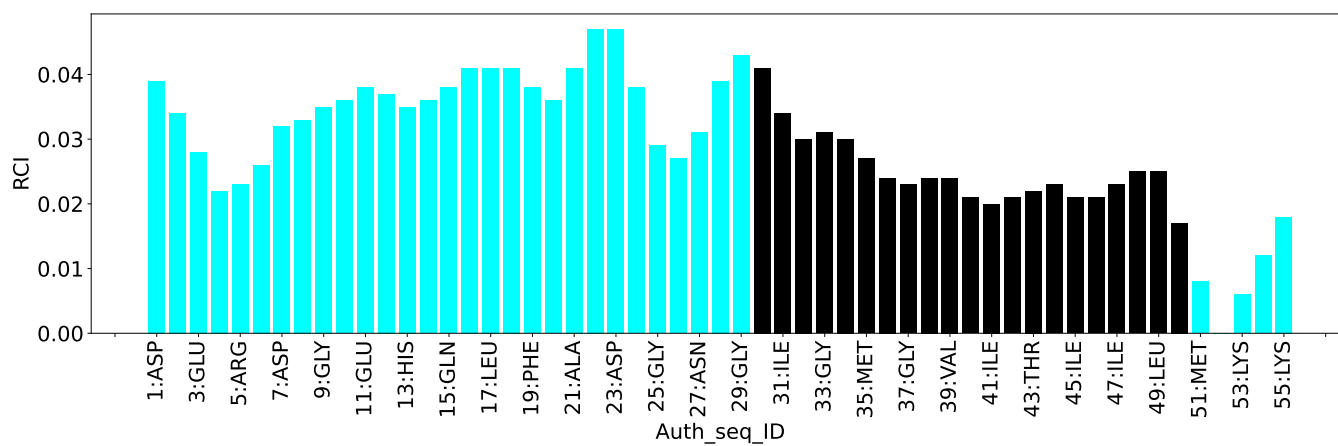
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	PRO	C	0.00	169.47 – 184.06	-121.2
1	A	52	PRO	CD	0.00	45.11 – 55.58	-48.1
1	A	52	PRO	CA	0.00	55.85 – 70.84	-42.3
1	A	52	PRO	CB	0.00	26.06 – 37.61	-27.6
1	A	52	PRO	N	0.00	108.67 – 162.11	-25.3
1	A	52	PRO	CG	0.00	21.69 – 32.72	-24.7
1	A	52	PRO	HA	0.00	2.78 – 6.00	-13.6
1	A	52	PRO	HD2	0.00	1.93 – 5.38	-10.6
1	A	52	PRO	HD3	0.00	1.76 – 5.48	-9.7
1	A	52	PRO	HG2	0.00	0.41 – 3.45	-6.3
1	A	52	PRO	HB2	0.00	0.37 – 3.78	-6.1
1	A	52	PRO	HG3	0.00	0.33 – 3.48	-6.0

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. 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	5
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	5
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.16
0.2-0.5 (Medium)	None	None
>0.5 (Large)	4.2	10.22

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 ⓘ

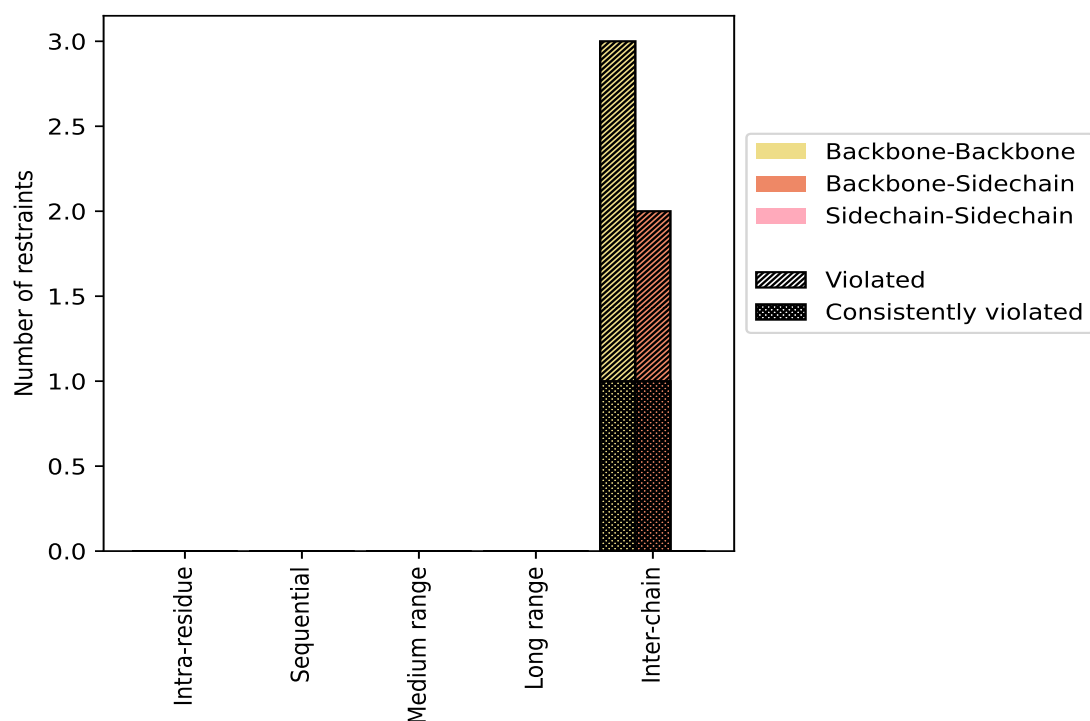
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	5	100.0	5	100.0	100.0	2	40.0	40.0
Backbone-Backbone	3	60.0	3	100.0	60.0	1	33.3	20.0
Backbone-Sidechain	2	40.0	2	100.0	40.0	1	50.0	20.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5	100.0	5	100.0	100.0	2	40.0	40.0
Backbone-Backbone	3	60.0	3	100.0	60.0	1	33.3	20.0
Backbone-Sidechain	2	40.0	2	100.0	40.0	1	50.0	20.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

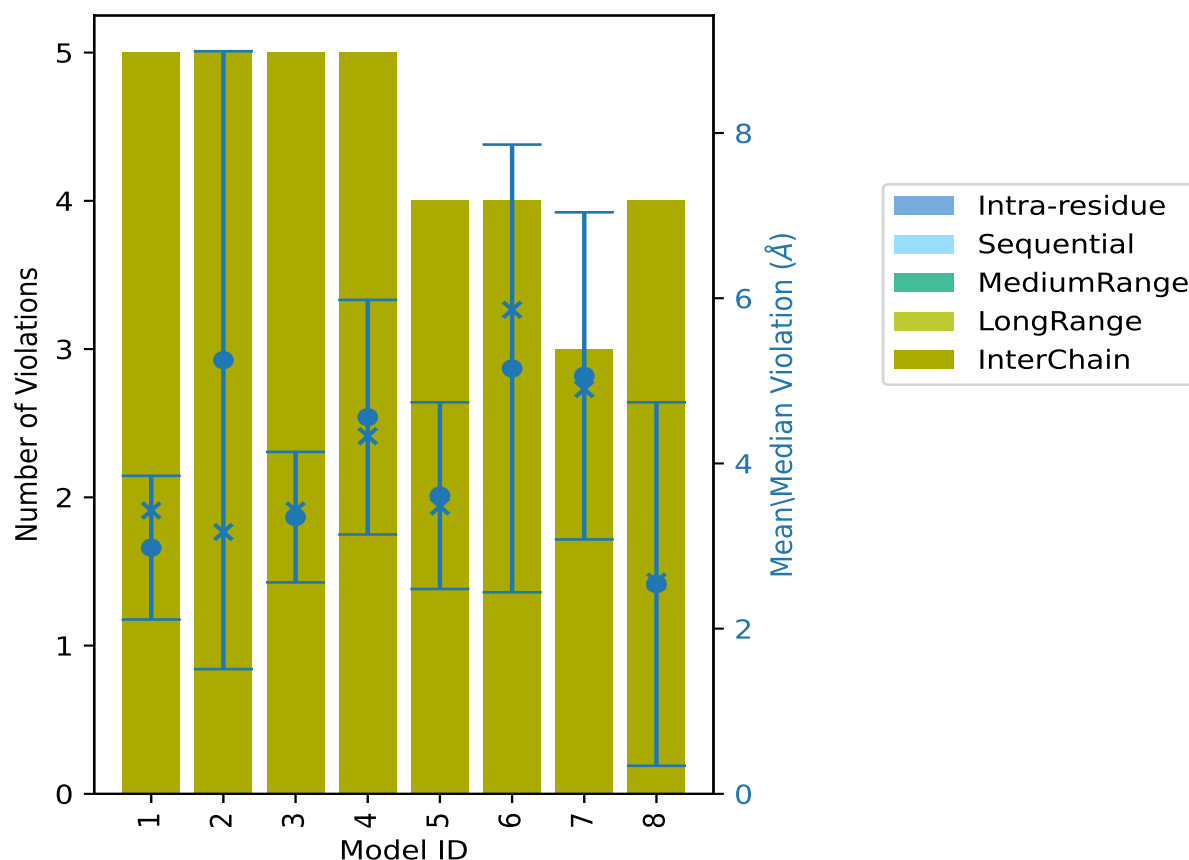
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	5	5	2.98	3.92	0.87	3.43
2	0	0	0	0	5	5	5.25	10.22	3.74	3.17
3	0	0	0	0	5	5	3.35	4.53	0.79	3.43
4	0	0	0	0	5	5	4.56	6.25	1.42	4.33
5	0	0	0	0	4	4	3.61	5.0	1.13	3.48
6	0	0	0	0	4	4	5.15	7.76	2.71	5.86
7	0	0	0	0	3	3	5.06	7.56	1.98	4.9
8	0	0	0	0	4	4	2.54	4.85	2.2	2.57

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, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	12.5
0	0	0	0	0	0	2	25.0
0	0	0	0	0	0	3	37.5
0	0	0	0	0	0	4	50.0
0	0	0	0	1	1	5	62.5
0	0	0	0	0	0	6	75.0

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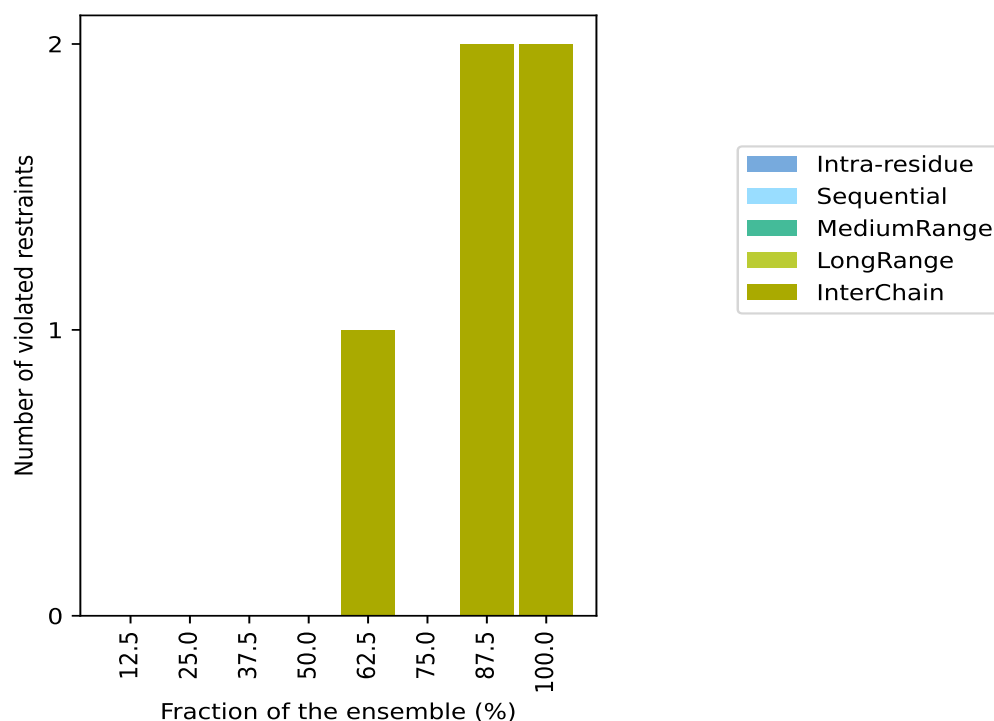
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	2	2	7	87.5
0	0	0	0	2	2	8	100.0

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

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

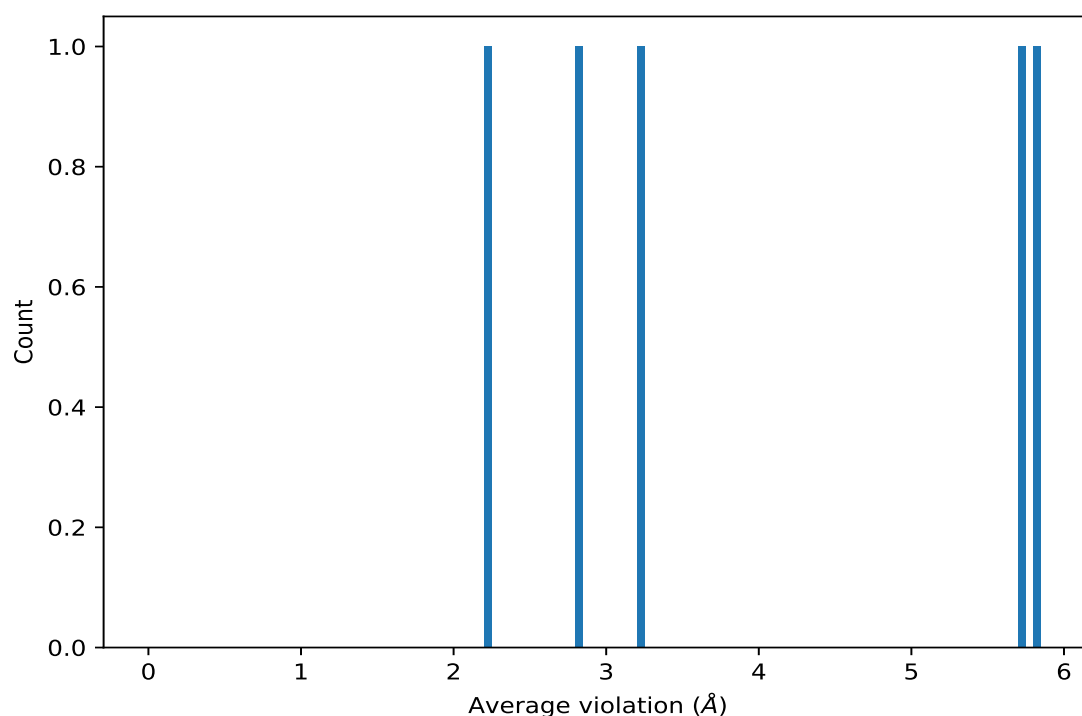
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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.

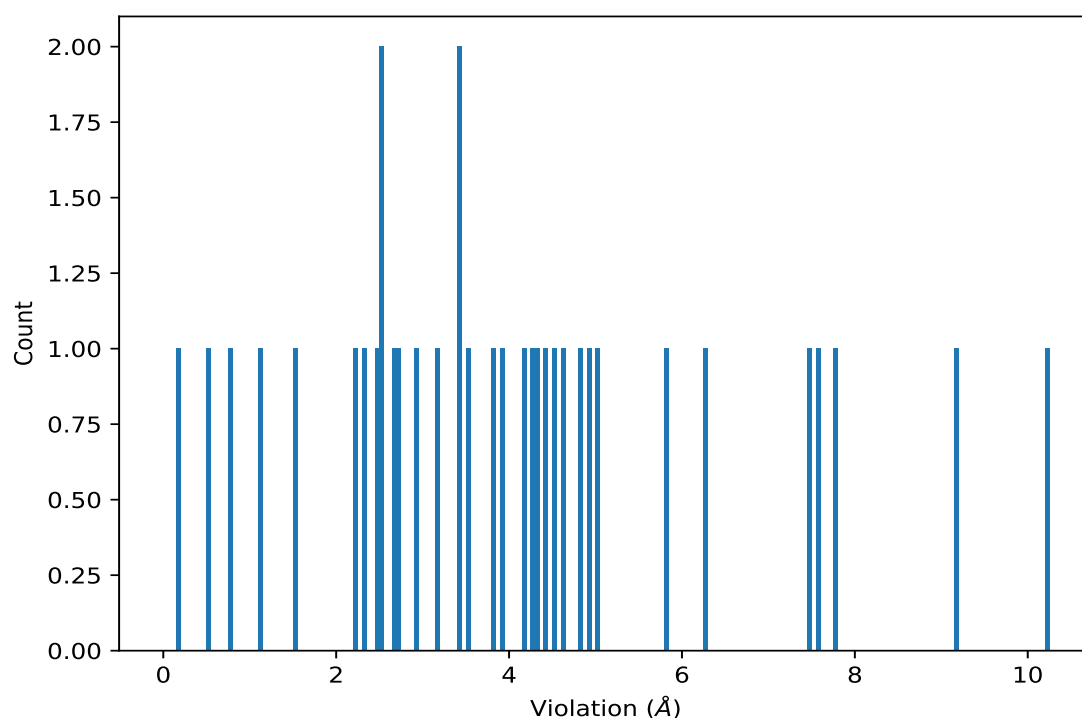
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	8	5.72	2.0	4.92
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	8	2.23	1.09	2.41
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	7	5.83	2.2	4.9
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	7	3.21	1.85	3.53
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	5	2.83	0.92	2.68

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	2	10.22
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	2	9.18
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	6	7.76
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	7	7.56
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	6	7.47
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	4	6.25
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	4	5.81
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	5	5.0
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	7	4.9
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	8	4.85
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	8	4.61
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	3	4.53
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	5	4.44
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	4	4.33
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	6	4.26
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	4	4.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	1	3.92
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	3	3.82
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	1	3.53
(1,2)	2:112:B:DAR:N	1:30:A:ALA:CB	1	3.43
(1,1)	2:112:B:DAR:N	1:27:A:ASN:ND2	3	3.43
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	2	3.17
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	2	2.91
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	7	2.72
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	3	2.68
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	5	2.52
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	1	2.5
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	5	2.49
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	3	2.31
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	4	2.24
(1,4)	2:112:B:DAR:N	1:18:A:VAL:N	1	1.5
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	6	1.11
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	2	0.76
(1,5)	2:112:B:DAR:N	1:20:A:PHE:N	8	0.53
(1,3)	2:112:B:DAR:N	1:17:A:LEU:N	8	0.16

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found