wwPDB NMR Structure Validation Summary Report

Dec 24, 2024 – 06:28 PM EST

PDB ID	:	2LVT
BMRB ID	:	18586
Title	:	Solution structure of Miz-1 zinc finger 9
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Deposited on	:	2012-07-11

This is a wwPDB NMR Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

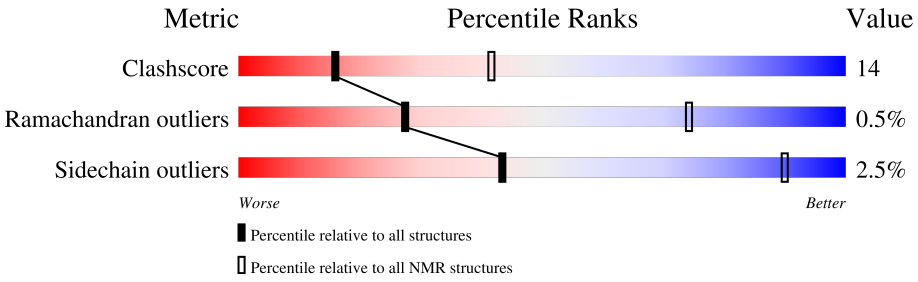
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	83	20% 6% 8% 65%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:33-A:54 (22)	0.33	1

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 9, 10, 11, 13, 14, 16, 20
2	3, 6, 7
3	5, 8, 12
4	15, 19
5	17, 18

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 437 atoms, of which 219 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger and BTB domain-containing protein 17.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	29	436	133	219	42	38	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13105

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

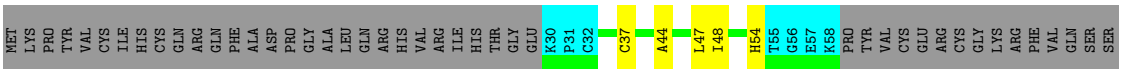
4 Residue-property plots (i)

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: Zinc finger and BTB domain-containing protein 17

Chain A:

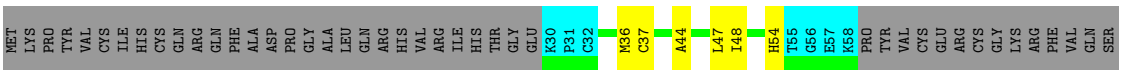


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Zinc finger and BTB domain-containing protein 17

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 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
ARIA	structure calculation	2.2
ARIA	refinement	2.2
CNS	structure calculation	1.21
CNS	refinement	1.21

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	877
Number of shifts mapped to atoms	288
Number of unparsed shifts	0
Number of shifts with mapping errors	589
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	166	165	165	5±2
All	All	3340	3300	3300	94

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 14.

5 of 26 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLN:HA	1:A:43:GLN:HE21	0.70	1.46	20	1
1:A:37:CYS:SG	1:A:39:LYS:HG2	0.67	2.29	6	1
1:A:36:MET:HG2	1:A:54:HIS:HB3	0.67	1.65	4	1
1:A:44:ALA:O	1:A:48:ILE:HG12	0.64	1.93	2	17
1:A:53:GLN:HE21	1:A:53:GLN:HA	0.63	1.53	13	3

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	22/83 (27%)	21±0 (94±2%)	1±1 (6±3%)	0±0 (0±1%)	27 74
All	All	440/1660 (27%)	412 (94%)	26 (6%)	2 (0%)	27 74

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	34	CYS	2

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	18/72 (25%)	18±1 (98±4%)	0±1 (2±4%)	43 90
All	All	360/1440 (25%)	351 (98%)	9 (2%)	43 90

All 5 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	53	GLN	3
1	A	33	GLN	2
1	A	39	LYS	2
1	A	52	ARG	1
1	A	43	GLN	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)

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

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

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	877
Number of shifts mapped to atoms	288
Number of unparsed shifts	0
Number of shifts with mapping errors	589
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 589) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	VAL	H	8.27	0.007	1
1	A	23	VAL	N	114.222	0.038	1
1	A	23	VAL	CA	65.99	0.054	1
1	A	23	VAL	CB	31.834	0.06	1
1	A	24	ARG	H	6.764	0.01	1
1	A	24	ARG	N	118.135	0.046	1
1	A	24	ARG	CA	57.94	0.0	1
1	A	24	ARG	CB	29.865	0.005	1
1	A	25	ILE	H	7.682	0.009	1
1	A	25	ILE	N	115.964	0.027	1
1	A	25	ILE	CA	62.939	0.017	1
1	A	25	ILE	CB	37.491	0.025	1
1	A	26	HIS	H	7.282	0.009	1
1	A	26	HIS	N	117.871	0.051	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	HIS	CA	55.107	0.077	1
1	A	26	HIS	CB	27.955	0.062	1
1	A	27	THR	H	7.534	0.014	1
1	A	27	THR	N	112.24	0.029	1
1	A	27	THR	CA	62.725	0.038	1
1	A	27	THR	CB	69.495	0.054	1
1	A	18	ALA	H	8.022	0.008	1
1	A	18	ALA	N	125.453	0.028	1
1	A	18	ALA	CA	54.562	0.027	1
1	A	18	ALA	CB	18.794	0.027	1
1	A	19	LEU	H	6.804	0.006	1
1	A	19	LEU	N	118.428	0.012	1
1	A	19	LEU	CA	57.723	0.029	1
1	A	19	LEU	CB	40.447	0.06	1
1	A	20	GLN	H	7.931	0.008	1
1	A	20	GLN	N	118.513	0.023	1
1	A	20	GLN	CA	58.675	0.009	1
1	A	20	GLN	CB	27.969	0.006	1
1	A	21	ARG	H	7.727	0.004	1
1	A	21	ARG	N	116.497	0.045	1
1	A	21	ARG	CA	58.956	0.09	1
1	A	21	ARG	CB	30.353	0.003	1
1	A	4	TYR	H	7.733	0.008	1
1	A	4	TYR	N	118.693	0.043	1
1	A	4	TYR	CA	57.954	0.034	1
1	A	4	TYR	CB	38.475	0.034	1
1	A	3	PRO	CA	63.467	0.033	1
1	A	3	PRO	CB	32.306	0.069	1
1	A	5	VAL	H	8.42	0.008	1
1	A	5	VAL	N	123.592	0.033	1
1	A	5	VAL	CA	60.269	0.012	1
1	A	5	VAL	CB	34.83	0.027	1
1	A	6	CYS	H	9.004	0.005	1
1	A	6	CYS	N	128.449	0.031	1
1	A	6	CYS	CA	59.271	0.045	1
1	A	6	CYS	CB	29.754	0.045	1
1	A	7	ILE	H	8.658	0.006	1
1	A	7	ILE	N	128.379	0.044	1
1	A	7	ILE	CA	63.258	0.023	1
1	A	7	ILE	CB	37.975	0.06	1
1	A	8	HIS	H	8.502	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	HIS	N	121.674	0.03	1
1	A	8	HIS	CA	57.836	0.054	1
1	A	8	HIS	CB	29.345	0.03	1
1	A	74	GLN	H	6.631	0.01	1
1	A	74	GLN	N	121.071	0.023	1
1	A	17	GLY	H	8.254	0.006	1
1	A	17	GLY	N	110.007	0.066	1
1	A	17	GLY	CA	46.69	0.027	1
1	A	16	PRO	CA	64.165	0.026	1
1	A	16	PRO	CB	31.085	0.022	1
1	A	75	LEU	H	6.652	0.007	1
1	A	75	LEU	N	121.285	0.038	1
1	A	75	LEU	CA	57.377	0.08	1
1	A	75	LEU	CB	40.208	0.069	1
1	A	74	GLN	CB	28.223	0.026	1
1	A	74	GLN	CA	57.752	0.08	1
1	A	76	ALA	H	7.88	0.009	1
1	A	76	ALA	N	120.443	0.028	1
1	A	76	ALA	CA	55.208	0.055	1
1	A	76	ALA	CB	17.548	0.033	1
1	A	77	ASN	H	7.443	0.005	1
1	A	77	ASN	N	115.335	0.049	1
1	A	77	ASN	CA	56.003	0.05	1
1	A	77	ASN	CB	38.701	0.063	1
1	A	78	HIS	H	7.419	0.008	1
1	A	78	HIS	N	119.301	0.045	1
1	A	78	HIS	CA	58.784	0.055	1
1	A	78	HIS	CB	28.529	0.027	1
1	A	79	ILE	H	8.253	0.012	1
1	A	79	ILE	N	116.732	0.04	1
1	A	79	ILE	CA	64.829	0.063	1
1	A	79	ILE	CB	37.947	0.025	1
1	A	80	ARG	H	7.295	0.008	1
1	A	80	ARG	N	119.229	0.053	1
1	A	80	ARG	CA	58.192	0.052	1
1	A	80	ARG	CB	29.9	0.004	1
1	A	9	CYS	H	7.942	0.007	1
1	A	9	CYS	N	115.764	0.035	1
1	A	9	CYS	CA	58.494	0.016	1
1	A	9	CYS	CB	32.209	0.03	1
1	A	10	GLN	H	8.191	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	GLN	N	116.329	0.021	1
1	A	10	GLN	CA	58.438	0.035	1
1	A	10	GLN	CB	25.356	0.013	1
1	A	11	ARG	H	7.844	0.007	1
1	A	11	ARG	N	121.213	0.028	1
1	A	11	ARG	CA	57.912	0.025	1
1	A	11	ARG	CB	31.307	0.048	1
1	A	12	GLN	H	7.86	0.007	1
1	A	12	GLN	N	119.072	0.031	1
1	A	12	GLN	CA	54.345	0.059	1
1	A	12	GLN	CB	31.148	0.069	1
1	A	13	PHE	H	8.888	0.011	1
1	A	13	PHE	N	119.084	0.026	1
1	A	13	PHE	CA	57.278	0.019	1
1	A	14	ALA	H	8.962	0.003	1
1	A	14	ALA	N	121.775	0.047	1
1	A	14	ALA	CA	53.149	0.044	1
1	A	14	ALA	CB	19.805	0.029	1
1	A	15	ASP	H	7.351	0.006	1
1	A	15	ASP	N	114.226	0.019	1
1	A	15	ASP	CA	51.23	0.058	1
1	A	15	ASP	CB	42.66	0.014	1
1	A	22	HIS	H	7.374	0.008	1
1	A	22	HIS	N	118.228	0.022	1
1	A	22	HIS	CA	59.068	0.032	1
1	A	22	HIS	CB	28.49	0.025	1
1	A	81	HIS	H	7.269	0.012	1
1	A	81	HIS	N	115.839	0.04	1
1	A	81	HIS	CA	54.913	0.013	1
1	A	81	HIS	CB	28.647	0.046	1
1	A	82	HIS	H	7.325	0.021	1
1	A	82	HIS	N	120.912	0.068	1
1	A	82	HIS	CA	58.009	0.02	1
1	A	82	HIS	CB	29.24	0.061	1
1	A	83	ASP	H	7.96	0.008	1
1	A	83	ASP	N	127.886	0.034	1
1	A	83	ASP	CA	55.889	0.023	1
1	A	83	ASP	CB	41.649	0.019	1
1	A	13	PHE	CB	43.35	0.034	1
1	A	60	TYR	H	8.103	0.012	1
1	A	60	TYR	N	119.458	0.041	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	TYR	CA	57.478	0.081	1
1	A	60	TYR	CB	38.062	0.067	1
1	A	59	PRO	CA	62.864	0.065	1
1	A	59	PRO	CB	32.179	0.045	1
1	A	61	VAL	H	8.236	0.013	1
1	A	61	VAL	N	123.692	0.043	1
1	A	61	VAL	CA	60.902	0.042	1
1	A	61	VAL	CB	34.808	0.042	1
1	A	62	CYS	H	8.837	0.008	1
1	A	62	CYS	N	128.744	0.025	1
1	A	62	CYS	CA	59.193	0.04	1
1	A	62	CYS	CB	29.875	0.037	1
1	A	63	GLU	H	9.397	0.008	1
1	A	63	GLU	N	132.308	0.023	1
1	A	63	GLU	CA	58.437	0.066	1
1	A	63	GLU	CB	29.567	0.076	1
1	A	64	ARG	H	8.73	0.004	1
1	A	64	ARG	N	120.08	0.027	1
1	A	64	ARG	CA	58.003	0.041	1
1	A	64	ARG	CB	30.365	0.019	1
1	A	65	CYS	H	8.139	0.006	1
1	A	65	CYS	N	115.27	0.027	1
1	A	65	CYS	CA	58.433	0.06	1
1	A	65	CYS	CB	32.677	0.058	1
1	A	66	GLY	H	8.26	0.007	1
1	A	66	GLY	N	113.667	0.023	1
1	A	66	GLY	CA	46.005	0.046	1
1	A	67	LYS	H	7.954	0.005	1
1	A	67	LYS	N	123.14	0.026	1
1	A	67	LYS	CA	58.348	0.017	1
1	A	67	LYS	CB	33.472	0.009	1
1	A	68	ARG	H	7.534	0.006	1
1	A	68	ARG	N	119.054	0.02	1
1	A	68	ARG	CA	54.302	0.064	1
1	A	68	ARG	CB	33.529	0.032	1
1	A	69	PHE	H	8.823	0.005	1
1	A	69	PHE	N	117.359	0.034	1
1	A	69	PHE	CA	56.798	0.011	1
1	A	69	PHE	CB	43.449	0.019	1
1	A	70	VAL	H	8.59	0.005	1
1	A	70	VAL	N	119.055	0.043	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	VAL	CA	64.666	0.057	1
1	A	70	VAL	CB	32.81	0.049	1
1	A	71	GLN	H	7.489	0.005	1
1	A	71	GLN	N	113.794	0.021	1
1	A	71	GLN	CA	53.641	0.004	1
1	A	71	GLN	CB	32.115	0.055	1
1	A	29	GLU	H	7.885	0.003	1
1	A	29	GLU	N	119.771	0.041	1
1	A	29	GLU	CA	56.901	0.02	1
1	A	29	GLU	CB	30.255	0.05	1
1	A	28	GLY	H	8.112	0.011	1
1	A	28	GLY	N	110.227	0.029	1
1	A	28	GLY	CA	45.243	0.046	1
1	A	3	PRO	C	176.021	.	1
1	A	4	TYR	C	174.332	.	1
1	A	5	VAL	C	174.141	.	1
1	A	6	CYS	C	177.123	.	1
1	A	7	ILE	C	175.653	.	1
1	A	8	HIS	C	176.78	.	1
1	A	9	CYS	C	174.989	.	1
1	A	10	GLN	C	174.724	.	1
1	A	11	ARG	C	174.125	.	1
1	A	12	GLN	C	175.08	.	1
1	A	13	PHE	C	174.976	.	1
1	A	14	ALA	C	176.59	.	1
1	A	16	PRO	C	178.827	.	1
1	A	17	GLY	C	175.863	.	1
1	A	18	ALA	C	180.54	.	1
1	A	19	LEU	C	176.841	.	1
1	A	20	GLN	C	178.29	.	1
1	A	21	ARG	C	178.324	.	1
1	A	22	HIS	C	176.672	.	1
1	A	23	VAL	C	176.856	.	1
1	A	24	ARG	C	178.102	.	1
1	A	25	ILE	C	177.015	.	1
1	A	26	HIS	C	175.472	.	1
1	A	27	THR	C	175.062	.	1
1	A	28	GLY	C	173.918	.	1
1	A	29	GLU	C	176.166	.	1
1	A	59	PRO	C	175.793	.	1
1	A	60	TYR	C	174.654	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	VAL	C	175.098	.	1
1	A	62	CYS	C	177.172	.	1
1	A	63	GLU	C	176.477	.	1
1	A	64	ARG	C	177.287	.	1
1	A	65	CYS	C	176.073	.	1
1	A	66	GLY	C	173.561	.	1
1	A	67	LYS	C	173.84	.	1
1	A	68	ARG	C	175.397	.	1
1	A	69	PHE	C	175.009	.	1
1	A	70	VAL	C	175.575	.	1
1	A	73	SER	C	176.771	.	1
1	A	74	GLN	C	178.884	.	1
1	A	75	LEU	C	177.083	.	1
1	A	76	ALA	C	180.212	.	1
1	A	77	ASN	C	176.329	.	1
1	A	78	HIS	C	176.836	.	1
1	A	79	ILE	C	178.108	.	1
1	A	80	ARG	C	176.59	.	1
1	A	81	HIS	C	174.531	.	1
1	A	82	HIS	C	174.904	.	1
1	A	73	SER	CA	60.413	0.069	1
1	A	73	SER	CB	61.588	0.056	1
1	A	3	PRO	CD	49.929	0.034	1
1	A	3	PRO	CG	26.582	0.016	1
1	A	7	ILE	CG1	26.684	0.059	1
1	A	7	ILE	CG2	17.445	0.056	1
1	A	7	ILE	CD1	13.836	0.09	1
1	A	10	GLN	CG	34.322	0.035	1
1	A	11	ARG	CD	43.622	.	1
1	A	11	ARG	CG	28.383	.	1
1	A	12	GLN	CG	33.754	0.048	1
1	A	16	PRO	CG	26.784	.	1
1	A	16	PRO	CD	49.894	0.036	1
1	A	19	LEU	CD1	23.328	.	1
1	A	20	GLN	CG	33.427	0.022	1
1	A	21	ARG	CD	43.232	0.012	1
1	A	21	ARG	CG	28.086	0.0	1
1	A	24	ARG	CD	43.555	.	1
1	A	24	ARG	CG	27.154	0.0	1
1	A	25	ILE	CG1	26.244	0.058	1
1	A	25	ILE	CG2	16.211	0.044	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	ILE	CD1	14.433	0.014	1
1	A	29	GLU	CG	36.152	0.019	1
1	A	59	PRO	CD	49.888	0.033	1
1	A	59	PRO	CG	26.838	0.005	1
1	A	63	GLU	CG	36.089	0.049	1
1	A	64	ARG	CD	42.845	0.002	1
1	A	64	ARG	CG	26.65	0.0	1
1	A	67	LYS	CE	42.139	.	1
1	A	67	LYS	CD	29.195	.	1
1	A	67	LYS	CG	26.519	0.001	1
1	A	68	ARG	CD	43.309	0.033	1
1	A	68	ARG	CG	28.285	0.033	1
1	A	70	VAL	CG2	22.039	0.01	2
1	A	70	VAL	CG1	21.854	0.058	2
1	A	74	GLN	CG	33.81	0.046	1
1	A	75	LEU	CG	27.029	.	1
1	A	75	LEU	CD1	26.039	0.019	2
1	A	75	LEU	CD2	22.969	0.014	2
1	A	80	ARG	CD	43.232	0.0	1
1	A	80	ARG	CG	27.179	0.0	1
1	A	79	ILE	CG1	28.859	0.068	1
1	A	79	ILE	CG2	17.556	0.07	1
1	A	79	ILE	CD1	13.609	0.03	1
1	A	4	TYR	HA	4.5	0.011	1
1	A	5	VAL	HA	4.634	0.009	1
1	A	6	CYS	HA	4.486	0.015	1
1	A	7	ILE	HA	3.929	0.015	1
1	A	8	HIS	HA	4.238	0.017	1
1	A	9	CYS	HA	5.041	0.018	1
1	A	10	GLN	HA	3.88	0.015	1
1	A	11	ARG	HA	3.935	0.013	1
1	A	12	GLN	HA	4.856	0.014	1
1	A	13	PHE	HA	4.487	0.003	1
1	A	15	ASP	HA	4.737	0.02	1
1	A	17	GLY	HA2	3.639	0.019	1
1	A	17	GLY	HA3	3.639	0.019	1
1	A	18	ALA	HA	3.841	0.022	1
1	A	19	LEU	HA	3.013	0.013	1
1	A	20	GLN	HA	3.79	0.014	1
1	A	21	ARG	HA	3.822	0.011	1
1	A	22	HIS	HA	4.131	0.016	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	ARG	HA	3.974	0.005	1
1	A	25	ILE	HA	3.844	0.011	1
1	A	26	HIS	HA	4.551	0.01	1
1	A	27	THR	HA	4.125	0.018	1
1	A	29	GLU	HA	4.048	0.015	1
1	A	76	ALA	HA	3.863	0.013	1
1	A	60	TYR	HA	4.426	0.018	1
1	A	61	VAL	HA	4.593	0.018	1
1	A	62	CYS	HA	4.496	0.013	1
1	A	63	GLU	HA	4.083	0.01	1
1	A	64	ARG	HA	4.142	0.015	1
1	A	65	CYS	HA	5.121	0.018	1
1	A	67	LYS	HA	3.816	0.016	1
1	A	68	ARG	HA	5.091	0.012	1
1	A	69	PHE	HA	4.67	0.02	1
1	A	70	VAL	HA	4.17	0.014	1
1	A	71	GLN	HA	4.758	0.01	1
1	A	74	GLN	HA	3.934	0.016	1
1	A	75	LEU	HA	3.06	0.008	1
1	A	77	ASN	HA	4.234	0.014	1
1	A	78	HIS	HA	4.133	0.015	1
1	A	79	ILE	HA	3.545	0.016	1
1	A	80	ARG	HA	3.91	0.01	1
1	A	81	HIS	HA	4.608	0.011	1
1	A	82	HIS	HA	3.981	0.015	1
1	A	83	ASP	HA	4.326	0.012	1
1	A	70	VAL	HB	2.203	0.008	1
1	A	70	VAL	HG21	1.085	0.003	2
1	A	70	VAL	HG22	1.085	0.003	2
1	A	70	VAL	HG23	1.085	0.003	2
1	A	70	VAL	HG11	1.02	0.007	2
1	A	70	VAL	HG12	1.02	0.007	2
1	A	70	VAL	HG13	1.02	0.007	2
1	A	7	ILE	HB	1.71	0.009	1
1	A	7	ILE	HG21	0.658	0.007	1
1	A	7	ILE	HG22	0.658	0.007	1
1	A	7	ILE	HG23	0.658	0.007	1
1	A	7	ILE	HD11	0.597	0.004	1
1	A	7	ILE	HD12	0.597	0.004	1
1	A	7	ILE	HD13	0.597	0.004	1
1	A	7	ILE	HG13	0.968	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ILE	HG12	0.968	0.007	1
1	A	65	CYS	HB3	3.352	0.013	1
1	A	65	CYS	HB2	2.823	0.015	1
1	A	60	TYR	HB2	2.776	0.017	1
1	A	60	TYR	HB3	2.776	0.017	1
1	A	16	PRO	HA	3.446	0.005	1
1	A	79	ILE	HB	1.857	0.015	1
1	A	79	ILE	HG13	1.662	0.013	2
1	A	79	ILE	HG12	1.347	0.016	2
1	A	79	ILE	HG21	0.908	0.009	1
1	A	79	ILE	HG22	0.908	0.009	1
1	A	79	ILE	HG23	0.908	0.009	1
1	A	79	ILE	HD11	0.885	0.015	1
1	A	79	ILE	HD12	0.885	0.015	1
1	A	79	ILE	HD13	0.885	0.015	1
1	A	68	ARG	HD3	3.128	0.004	2
1	A	68	ARG	HD2	3.015	0.014	2
1	A	68	ARG	HB3	1.671	0.008	2
1	A	68	ARG	HB2	1.314	0.01	2
1	A	12	GLN	HG3	2.255	0.016	2
1	A	12	GLN	HG2	2.031	0.01	2
1	A	12	GLN	HB3	1.758	0.005	2
1	A	12	GLN	HB2	1.63	0.013	2
1	A	71	GLN	HG3	2.304	0.01	2
1	A	71	GLN	HG2	2.262	0.011	2
1	A	71	GLN	HB2	2.166	0.003	1
1	A	71	GLN	HB3	1.595	0.019	1
1	A	71	GLN	CG	33.638	0.0	1
1	A	83	ASP	HB3	2.597	0.004	2
1	A	83	ASP	HB2	2.512	0.003	2
1	A	15	ASP	HB3	2.69	0.013	2
1	A	15	ASP	HB2	2.565	0.014	2
1	A	25	ILE	HB	1.589	0.009	1
1	A	25	ILE	HG13	0.763	0.018	1
1	A	25	ILE	HG12	0.763	0.018	1
1	A	25	ILE	HG21	0.455	0.005	1
1	A	25	ILE	HG22	0.455	0.005	1
1	A	25	ILE	HG23	0.455	0.005	1
1	A	25	ILE	HD11	0.544	0.006	1
1	A	25	ILE	HD12	0.544	0.006	1
1	A	25	ILE	HD13	0.544	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	ALA	HB1	1.497	0.011	1
1	A	18	ALA	HB2	1.497	0.011	1
1	A	18	ALA	HB3	1.497	0.011	1
1	A	14	ALA	HA	4.432	0.014	1
1	A	14	ALA	HB1	1.444	0.01	1
1	A	14	ALA	HB2	1.444	0.01	1
1	A	14	ALA	HB3	1.444	0.01	1
1	A	27	THR	HB	4.156	0.007	1
1	A	27	THR	HG21	1.069	0.019	1
1	A	27	THR	HG22	1.069	0.019	1
1	A	27	THR	HG23	1.069	0.019	1
1	A	4	TYR	HB3	2.861	0.004	2
1	A	4	TYR	HB2	2.734	0.011	2
1	A	5	VAL	HB	1.712	0.011	1
1	A	5	VAL	HG21	0.653	0.012	2
1	A	5	VAL	HG22	0.653	0.012	2
1	A	5	VAL	HG23	0.653	0.012	2
1	A	5	VAL	HG11	0.64	0.011	2
1	A	5	VAL	HG12	0.64	0.011	2
1	A	5	VAL	HG13	0.64	0.011	2
1	A	8	HIS	HB3	2.231	0.015	1
1	A	8	HIS	HB2	1.802	0.011	1
1	A	10	GLN	HG2	2.115	0.013	1
1	A	10	GLN	HG3	2.115	0.013	1
1	A	10	GLN	HB3	2.333	0.003	2
1	A	10	GLN	HB2	2.189	0.003	2
1	A	11	ARG	HD3	3.001	0.011	2
1	A	11	ARG	HB3	1.383	0.008	2
1	A	11	ARG	HB2	1.219	0.015	2
1	A	66	GLY	HA3	4.117	0.013	2
1	A	66	GLY	HA2	3.609	0.017	2
1	A	19	LEU	CD2	23.328	.	1
1	A	19	LEU	HB3	1.731	0.011	1
1	A	19	LEU	HB2	1.039	0.006	1
1	A	20	GLN	HG3	2.288	0.004	2
1	A	20	GLN	HG2	2.21	0.002	2
1	A	20	GLN	HB3	2.045	0.013	2
1	A	20	GLN	HB2	2.027	0.014	2
1	A	22	HIS	HB3	2.911	0.011	1
1	A	22	HIS	HB2	2.723	0.014	1
1	A	23	VAL	CG1	21.94	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	VAL	CG2	21.94	0.03	1
1	A	23	VAL	HA	3.494	0.018	1
1	A	23	VAL	HB	2.243	0.012	1
1	A	23	VAL	HG21	1.232	0.009	1
1	A	23	VAL	HG22	1.232	0.009	1
1	A	23	VAL	HG23	1.232	0.009	1
1	A	23	VAL	HG11	1.232	0.009	1
1	A	23	VAL	HG12	1.232	0.009	1
1	A	23	VAL	HG13	1.232	0.009	1
1	A	26	HIS	HB3	2.624	0.011	2
1	A	26	HIS	HB2	2.524	0.007	2
1	A	29	GLU	HB3	1.893	0.004	2
1	A	29	GLU	HB2	1.842	0.018	2
1	A	29	GLU	HG3	2.115	0.01	2
1	A	29	GLU	HG2	2.169	0.006	2
1	A	9	CYS	HB3	3.346	0.014	2
1	A	9	CYS	HB2	2.745	0.012	2
1	A	61	VAL	CG1	21.069	0.015	1
1	A	61	VAL	CG2	21.069	0.015	1
1	A	61	VAL	HB	1.71	0.014	1
1	A	61	VAL	HG21	0.658	0.011	2
1	A	61	VAL	HG22	0.658	0.011	2
1	A	61	VAL	HG23	0.658	0.011	2
1	A	61	VAL	HG11	0.615	0.012	2
1	A	61	VAL	HG12	0.615	0.012	2
1	A	61	VAL	HG13	0.615	0.012	2
1	A	5	VAL	CG1	20.921	.	1
1	A	5	VAL	CG2	20.921	.	1
1	A	62	CYS	HB3	3.281	0.015	1
1	A	62	CYS	HB2	2.757	0.021	1
1	A	6	CYS	HB3	3.281	0.015	1
1	A	6	CYS	HB2	2.747	0.016	1
1	A	63	GLU	HG3	2.248	0.012	1
1	A	63	GLU	HG2	2.245	0.014	1
1	A	63	GLU	HB3	2.066	0.002	2
1	A	63	GLU	HB2	1.991	0.008	2
1	A	73	SER	HA	3.957	0.005	1
1	A	73	SER	HB2	3.727	0.01	1
1	A	73	SER	HB3	3.727	0.01	1
1	A	74	GLN	HG2	2.414	0.003	1
1	A	74	GLN	HG3	2.414	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	GLN	HB2	2.342	0.007	1
1	A	74	GLN	HB3	1.945	0.011	1
1	A	77	ASN	HB2	2.644	0.015	1
1	A	77	ASN	HB3	2.644	0.015	1
1	A	82	HIS	HB2	3.12	0.044	1
1	A	82	HIS	HB3	2.885	0.013	1
1	A	28	GLY	HA3	3.813	0.003	2
1	A	28	GLY	HA2	3.879	0.007	2
1	A	59	PRO	HA	4.229	0.01	1
1	A	59	PRO	HD3	3.604	0.01	2
1	A	59	PRO	HD2	3.455	0.006	2
1	A	59	PRO	HB3	1.929	0.009	2
1	A	59	PRO	HB2	1.324	0.01	2
1	A	59	PRO	HG3	1.761	0.01	2
1	A	59	PRO	HG2	1.624	0.003	2
1	A	75	LEU	HB3	1.741	0.01	1
1	A	75	LEU	HB2	1.035	0.012	1
1	A	75	LEU	HD21	0.895	0.009	2
1	A	75	LEU	HD22	0.895	0.009	2
1	A	75	LEU	HD23	0.895	0.009	2
1	A	75	LEU	HD11	0.956	0.004	2
1	A	75	LEU	HD12	0.956	0.004	2
1	A	75	LEU	HD13	0.956	0.004	2
1	A	68	ARG	HG3	1.249	0.007	2
1	A	68	ARG	HG2	1.607	0.006	2
1	A	3	PRO	HA	4.187	0.013	1
1	A	3	PRO	HD3	3.667	0.022	2
1	A	3	PRO	HD2	3.596	0.006	2
1	A	3	PRO	HG3	1.743	0.028	2
1	A	3	PRO	HG2	1.551	0.009	2
1	A	3	PRO	HB3	1.904	0.011	2
1	A	3	PRO	HB2	1.233	0.003	2
1	A	69	PHE	HB3	3.374	0.013	1
1	A	69	PHE	HB2	2.458	0.016	1
1	A	76	ALA	HB1	1.247	0.014	1
1	A	76	ALA	HB2	1.247	0.014	1
1	A	76	ALA	HB3	1.247	0.014	1
1	A	78	HIS	HB3	3.154	0.017	1
1	A	78	HIS	HB2	2.737	0.013	1
1	A	81	HIS	HB3	3.157	0.026	2
1	A	81	HIS	HB2	2.717	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ARG	HD2	2.789	0.007	2
1	A	13	PHE	HB3	3.133	0.012	1
1	A	13	PHE	HB2	2.566	0.015	1
1	A	16	PRO	HD3	3.614	0.063	2
1	A	16	PRO	HD2	3.075	0.01	2
1	A	21	ARG	HD3	3.154	0.004	2
1	A	21	ARG	HD2	3.01	0.003	2
1	A	21	ARG	HB3	1.72	0.004	2
1	A	21	ARG	HB2	1.661	0.006	2
1	A	67	LYS	HE3	2.828	0.009	2
1	A	67	LYS	HE2	2.784	0.015	2
1	A	82	HIS	CE1	142.684	.	1
1	A	82	HIS	HE1	7.907	0.001	1
1	A	26	HIS	CE1	142.684	.	1
1	A	26	HIS	HE1	7.93	0.006	1
1	A	22	HIS	CD2	130.313	0.0	1
1	A	22	HIS	HD2	6.848	0.008	1
1	A	78	HIS	CD2	130.312	0.001	1
1	A	78	HIS	HD2	7.003	0.006	1
1	A	19	LEU	HD21	0.879	0.023	2
1	A	19	LEU	HD22	0.879	0.023	2
1	A	19	LEU	HD23	0.879	0.023	2
1	A	19	LEU	HD11	0.791	0.011	2
1	A	19	LEU	HD12	0.791	0.011	2
1	A	19	LEU	HD13	0.791	0.011	2
1	A	10	GLN	HE22	7.092	0.003	1
1	A	10	GLN	HE21	6.363	0.004	1
1	A	10	GLN	NE2	111.99	0.022	1
1	A	12	GLN	HE22	7.488	0.003	1
1	A	12	GLN	HE21	6.637	0.008	1
1	A	12	GLN	NE2	111.271	0.003	1
1	A	26	HIS	CD2	131.261	0.018	1
1	A	26	HIS	HD2	6.57	0.006	1
1	A	82	HIS	CD2	129.375	.	1
1	A	82	HIS	HD2	6.187	0.003	1
1	A	4	TYR	HD1	6.878	0.009	3
1	A	4	TYR	HD2	6.878	0.009	3
1	A	13	PHE	HD1	7.031	0.002	3
1	A	13	PHE	HD2	7.031	0.002	3
1	A	13	PHE	CD1	135.106	0.013	3
1	A	13	PHE	CD2	135.106	0.013	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	PHE	HD1	6.964	0.009	3
1	A	69	PHE	HD2	6.964	0.009	3
1	A	69	PHE	CD1	135.38	0.033	3
1	A	69	PHE	CD2	135.38	0.033	3
1	A	60	TYR	HD1	6.897	0.004	3
1	A	60	TYR	HD2	6.897	0.004	3
1	A	60	TYR	CD1	136.109	0.038	3
1	A	60	TYR	CD2	136.109	0.038	3
1	A	4	TYR	CD1	136.107	0.009	3
1	A	4	TYR	CD2	136.107	0.009	3
1	A	77	ASN	HD22	7.546	0.002	1
1	A	77	ASN	HD21	6.87	0.005	1
1	A	77	ASN	ND2	112.938	0.027	1
1	A	11	ARG	HG2	1.724	0.011	1
1	A	11	ARG	HG3	1.724	0.011	1
1	A	21	ARG	HG3	1.36	0.008	1
1	A	21	ARG	HG2	1.36	0.008	1
1	A	24	ARG	HD2	3.061	0.006	1
1	A	24	ARG	HD3	3.067	0.002	1
1	A	24	ARG	HB2	1.741	0.0	1
1	A	24	ARG	HB3	1.741	0.0	1
1	A	24	ARG	HG3	1.655	0.003	2
1	A	24	ARG	HG2	1.55	0.003	2
1	A	64	ARG	HD3	2.601	0.006	2
1	A	64	ARG	HD2	2.434	0.009	2
1	A	64	ARG	HB3	1.428	0.003	2
1	A	64	ARG	HB2	1.306	0.003	2
1	A	64	ARG	HG3	1.386	0.003	2
1	A	64	ARG	HG2	1.263	0.004	2
1	A	67	LYS	HG3	0.904	0.007	2
1	A	67	LYS	HG2	1.297	0.003	2
1	A	67	LYS	HB3	1.084	0.003	2
1	A	67	LYS	HB2	1.325	0.005	2
1	A	67	LYS	HD2	1.372	0.002	1
1	A	67	LYS	HD3	1.372	0.002	1
1	A	75	LEU	HG	1.501	0.006	1
1	A	80	ARG	HD3	3.021	0.005	1
1	A	80	ARG	HD2	3.019	0.006	1
1	A	80	ARG	HB3	1.657	0.002	2
1	A	80	ARG	HB2	1.593	0.003	2
1	A	80	ARG	HG3	1.417	0.016	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	ARG	HG2	1.274	0.007	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	80	-0.46 ± 0.53	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	75	0.52 ± 0.55	None needed (imprecise)
$^{13}C'$	74	-0.33 ± 0.55	None needed (< 0.5 ppm)
^{15}N	74	0.55 ± 1.24	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 234 atoms were assigned a chemical shift out of a possible 291. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	108/111 (97%)	44/45 (98%)	43/44 (98%)	21/22 (95%)
Sidechain	116/156 (74%)	79/103 (77%)	37/46 (80%)	0/7 (0%)
Aromatic	10/24 (42%)	5/13 (38%)	5/9 (56%)	0/2 (0%)
Overall	234/291 (80%)	128/161 (80%)	85/99 (86%)	21/31 (68%)

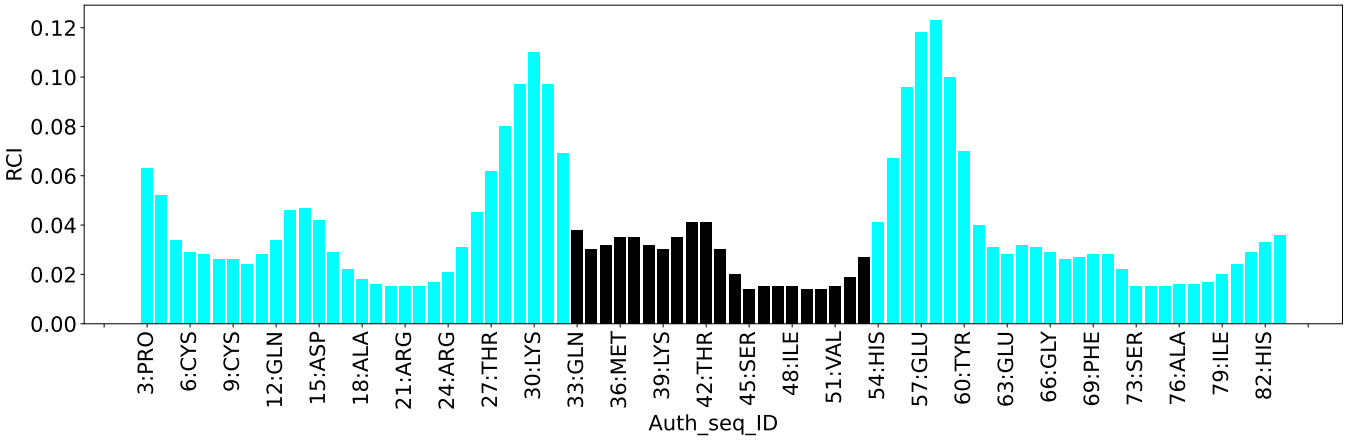
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
3:PRO
6:CYS
9:CYS
12:GLN
15:ASP
18:ALA
21:ARG
24:ARG
27:THR
30:LYS
33:GLN
36:MET
39:LYS
42:THR
45:SER
48:ILE
51:VAL
54:HIS
57:GLU
60:TYR
63:GLU
66:GLY
69:PHE
73:SER
76:ALA
79:ILE
82:HIS
Auth_seq_ID

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	438
Intra-residue (|i-j|=0)	235
Sequential (|i-j|=1)	120
Medium range (|i-j|>1 and |i-j|<5)	54
Long range (|i-j|≥5)	29
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	60
Number of unmapped restraints	0
Number of restraints per residue	5.9
Number of long range restraints per residue[1]	0.3

[1]Long 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)	3.7	0.2
0.2-0.5 (Medium)	4.3	0.5
>0.5 (Large)	4.4	2.11

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.1	4.21
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

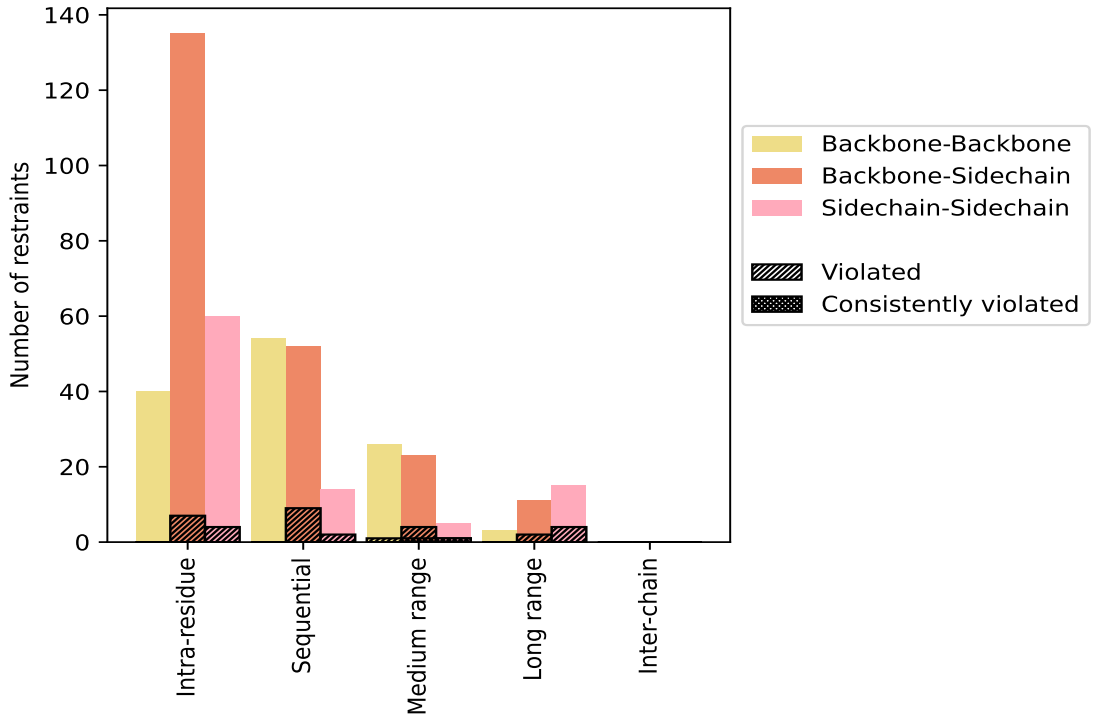
9.1 Summary of distance violations (i)

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)	235	53.7	11	4.7	2.5	0	0.0	0.0
Backbone-Backbone	40	9.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	135	30.8	7	5.2	1.6	0	0.0	0.0
Sidechain-Sidechain	60	13.7	4	6.7	0.9	0	0.0	0.0
Sequential (|i-j|=1)	120	27.4	11	9.2	2.5	0	0.0	0.0
Backbone-Backbone	54	12.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	52	11.9	9	17.3	2.1	0	0.0	0.0
Sidechain-Sidechain	14	3.2	2	14.3	0.5	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	54	12.3	6	11.1	1.4	2	3.7	0.5
Backbone-Backbone	26	5.9	1	3.8	0.2	0	0.0	0.0
Backbone-Sidechain	23	5.3	4	17.4	0.9	1	4.3	0.2
Sidechain-Sidechain	5	1.1	1	20.0	0.2	1	20.0	0.2
Long range (|i-j|≥5)	29	6.6	6	20.7	1.4	0	0.0	0.0
Backbone-Backbone	3	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	11	2.5	2	18.2	0.5	0	0.0	0.0
Sidechain-Sidechain	15	3.4	4	26.7	0.9	0	0.0	0.0
Inter-chain	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
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	438	100.0	34	7.8	7.8	2	0.5	0.5
Backbone-Backbone	123	28.1	1	0.8	0.2	0	0.0	0.0
Backbone-Sidechain	221	50.5	22	10.0	5.0	1	0.5	0.2
Sidechain-Sidechain	94	21.5	11	11.7	2.5	1	1.1	0.2

[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



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

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	2	0	4	2	0	8	0.53	1.56	0.53	0.26
2	3	3	4	2	0	12	0.55	1.34	0.47	0.3
3	3	1	5	4	0	13	0.54	1.7	0.5	0.36
4	4	1	4	3	0	12	0.54	1.71	0.43	0.41
5	3	1	4	3	0	11	0.44	1.69	0.42	0.3
6	3	0	3	2	0	8	0.62	2.0	0.63	0.32
7	5	5	4	3	0	17	0.5	1.79	0.53	0.15
8	3	4	3	3	0	13	0.68	1.69	0.5	0.51
9	4	5	5	2	0	16	0.54	1.94	0.53	0.32
10	4	5	5	3	0	17	0.51	2.11	0.53	0.34

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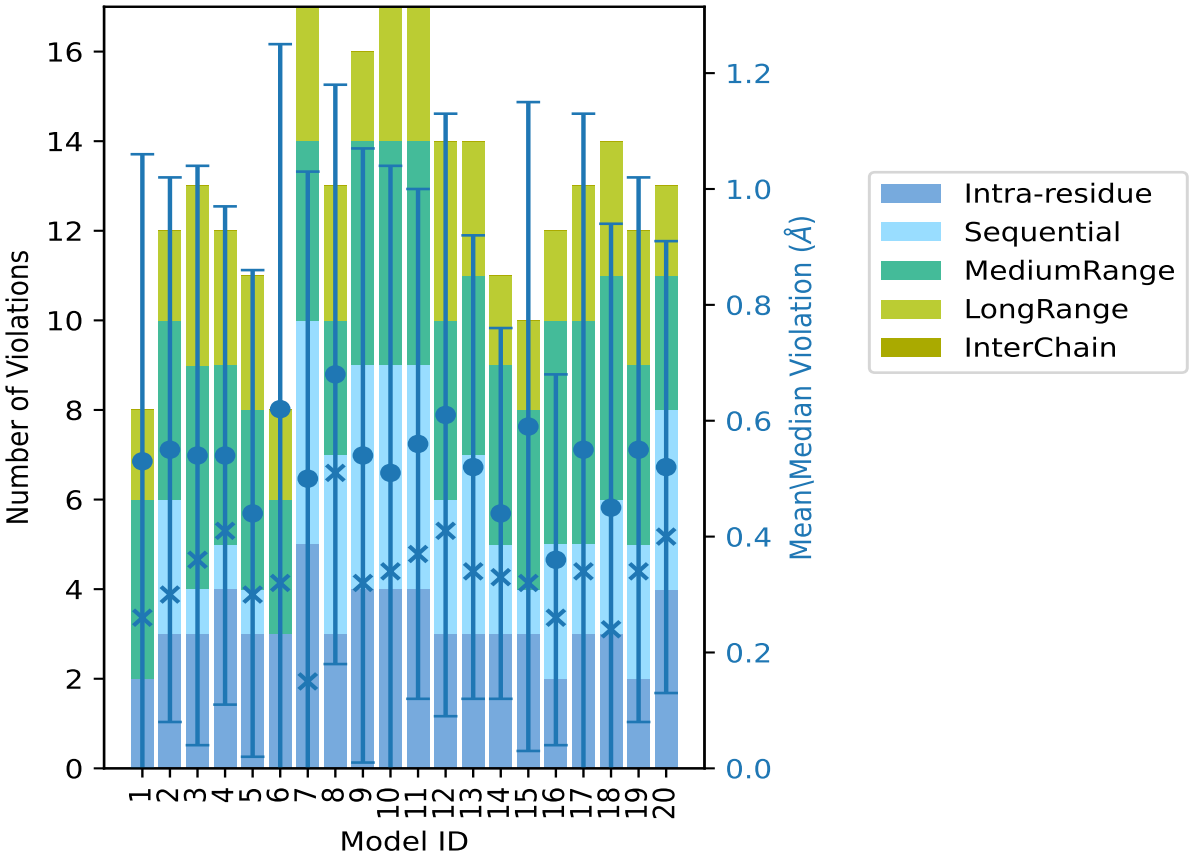
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	5	5	3	0	17	0.56	1.6	0.44	0.37
12	3	3	4	4	0	14	0.61	1.76	0.52	0.41
13	3	4	4	3	0	14	0.52	1.29	0.4	0.34
14	3	2	4	2	0	11	0.44	1.25	0.32	0.33
15	3	1	4	2	0	10	0.59	1.95	0.56	0.32
16	2	3	5	2	0	12	0.36	1.26	0.32	0.26
17	3	2	5	3	0	13	0.55	1.96	0.58	0.34
18	3	3	5	3	0	14	0.45	1.73	0.49	0.24
19	2	3	4	3	0	12	0.55	1.54	0.47	0.34
20	4	4	3	2	0	13	0.52	1.61	0.39	0.4

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

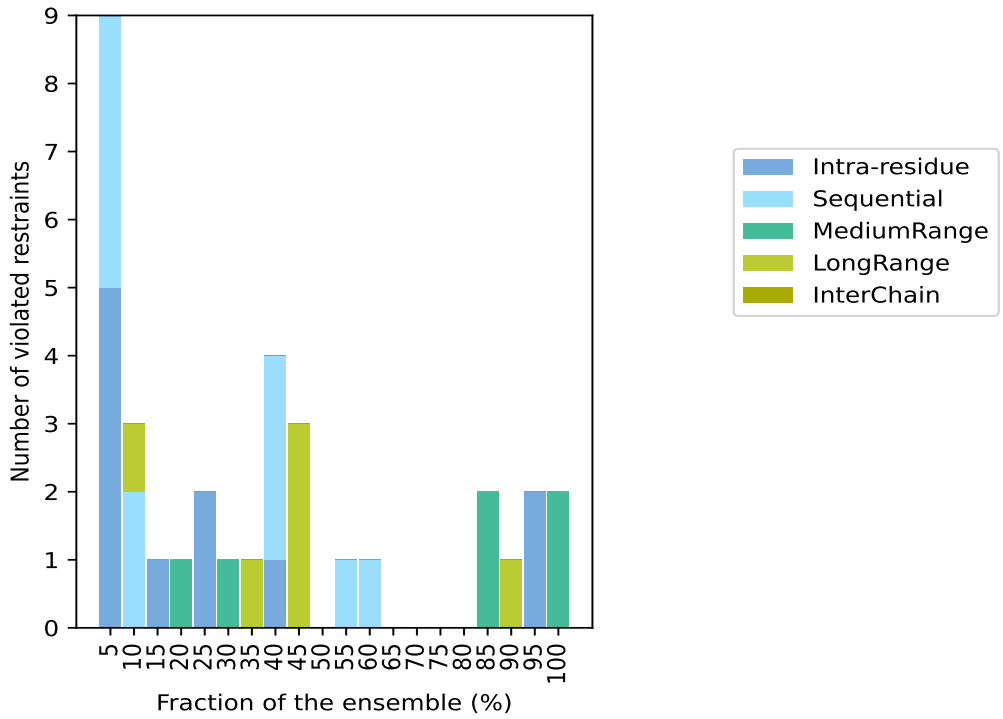
9.3 Distance violation statistics for the ensemble (i)

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, 404(IR:224, SQ:109, MR:48, LR:23, 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]	%
5	4	0	0	0	9	1	5.0
0	2	0	1	0	3	2	10.0
1	0	0	0	0	1	3	15.0
0	0	1	0	0	1	4	20.0
2	0	0	0	0	2	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	1	0	1	7	35.0
1	3	0	0	0	4	8	40.0
0	0	0	3	0	3	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	0	0	1	11	55.0
0	1	0	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	2	0	0	2	17	85.0
0	0	0	1	0	1	18	90.0
2	0	0	0	0	2	19	95.0
0	0	2	0	0	2	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

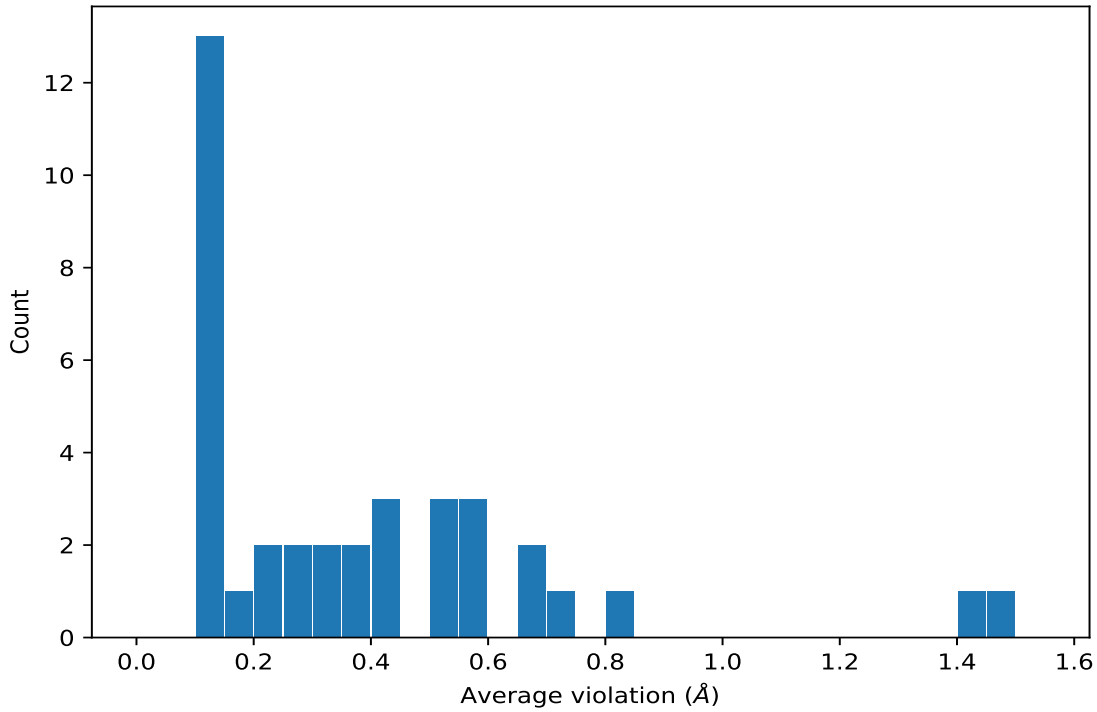
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

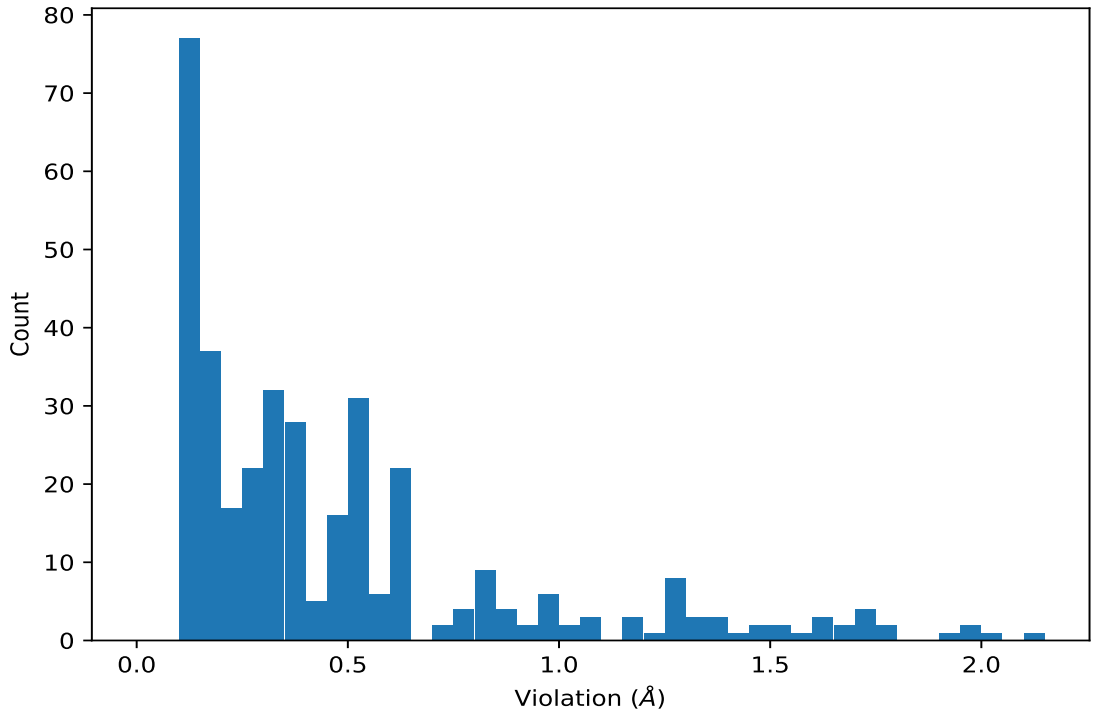
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,433)	1:45:A:SER:HA	1:47:A:LEU:HB2	20	1.47	0.19	1.39
(1,131)	1:44:A:ALA:HB1	1:47:A:LEU:HB2	20	0.44	0.22	0.36
(1,131)	1:44:A:ALA:HB2	1:47:A:LEU:HB2	20	0.44	0.22	0.36
(1,131)	1:44:A:ALA:HB3	1:47:A:LEU:HB2	20	0.44	0.22	0.36
(1,283)	1:53:A:GLN:H	1:53:A:GLN:HB3	19	0.35	0.01	0.35
(1,92)	1:53:A:GLN:HG3	1:53:A:GLN:HA	19	0.31	0.04	0.32
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	18	1.43	0.51	1.53
(1,152)	1:48:A:ILE:HG13	1:44:A:ALA:HA	17	0.21	0.05	0.19
(1,67)	1:34:A:CYS:HB2	1:37:A:CYS:H	17	0.16	0.03	0.16
(1,15)	1:56:A:GLY:HA2	1:57:A:GLU:HB2	12	0.68	0.5	0.6
(1,407)	1:56:A:GLY:HA2	1:57:A:GLU:HG3	11	0.84	0.3	0.87
(1,217)	1:35:A:VAL:H	1:47:A:LEU:HD11	9	0.6	0.11	0.6

[1]Number of violated models, [2]Standard 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 provides the 10 worst performing restraints, sorted by the violation 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)
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	10	2.11
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	6	2.0
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	17	1.96
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	15	1.95
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	9	1.94
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	7	1.79
(1,416)	1:38:A:GLY:HA3	1:33:A:GLN:HB2	12	1.76
(1,433)	1:45:A:SER:HA	1:47:A:LEU:HB2	17	1.74
(1,433)	1:45:A:SER:HA	1:47:A:LEU:HB2	18	1.73
(1,433)	1:45:A:SER:HA	1:47:A:LEU:HB2	4	1.71

10 Dihedral-angle violation analysis

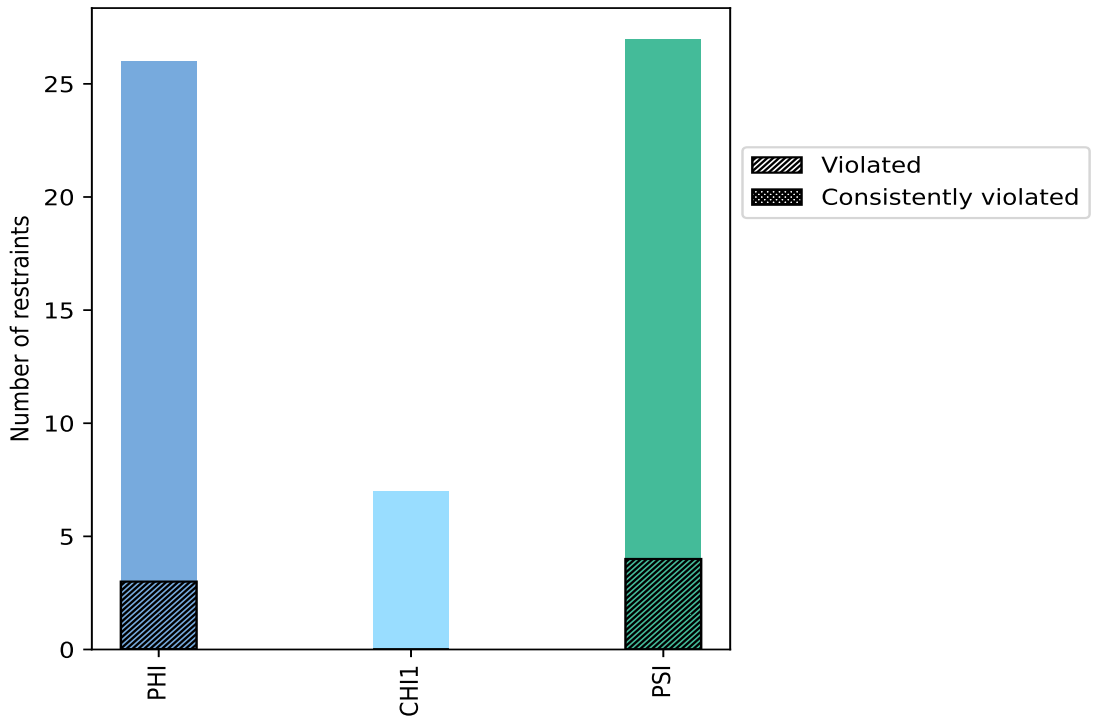
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	26	43.3	3	11.5	5.0	0	0.0	0.0
CHI1	7	11.7	0	0.0	0.0	0	0.0	0.0
PSI	27	45.0	4	14.8	6.7	0	0.0	0.0
Total	60	100.0	7	11.7	11.7	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



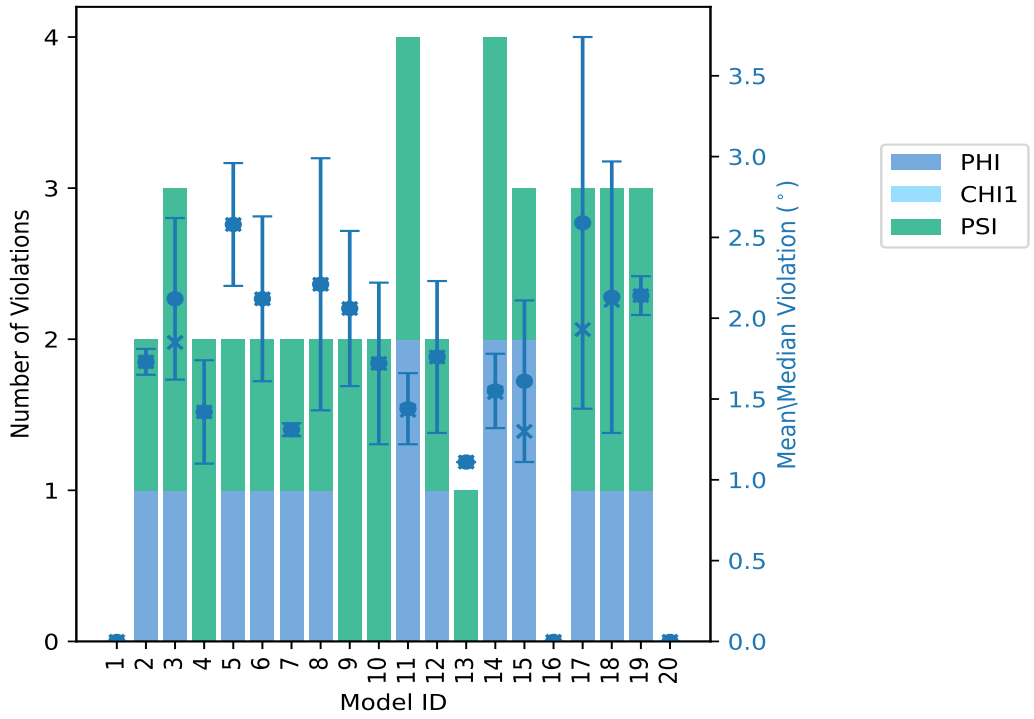
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	CHI1	PSI	Total				
1	0	0	0	0	0.0	0.0	0.0	0.0
2	1	0	1	2	1.73	1.81	0.08	1.73
3	1	0	2	3	2.12	2.83	0.5	1.85
4	0	0	2	2	1.42	1.74	0.32	1.42
5	1	0	1	2	2.58	2.96	0.38	2.58
6	1	0	1	2	2.12	2.63	0.51	2.12
7	1	0	1	2	1.31	1.35	0.04	1.31
8	1	0	1	2	2.21	2.99	0.78	2.21
9	0	0	2	2	2.06	2.54	0.48	2.06
10	0	0	2	2	1.72	2.22	0.5	1.72
11	2	0	2	4	1.44	1.71	0.22	1.43
12	1	0	1	2	1.76	2.22	0.47	1.76
13	0	0	1	1	1.11	1.11	0.0	1.11
14	2	0	2	4	1.55	1.8	0.23	1.54
15	2	0	1	3	1.61	2.31	0.5	1.3
16	0	0	0	0	0.0	0.0	0.0	0.0
17	1	0	2	3	2.59	4.21	1.15	1.93
18	1	0	2	3	2.13	3.17	0.84	2.11
19	1	0	2	3	2.14	2.29	0.12	2.14
20	0	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
1	0	0	1	1	5.0
0	0	2	2	2	10.0
0	0	0	0	3	15.0
0	0	0	0	4	20.0
0	0	0	0	5	25.0
1	0	0	1	6	30.0
0	0	1	1	7	35.0
0	0	0	0	8	40.0
1	0	0	1	9	45.0
0	0	0	0	10	50.0
0	0	0	0	11	55.0

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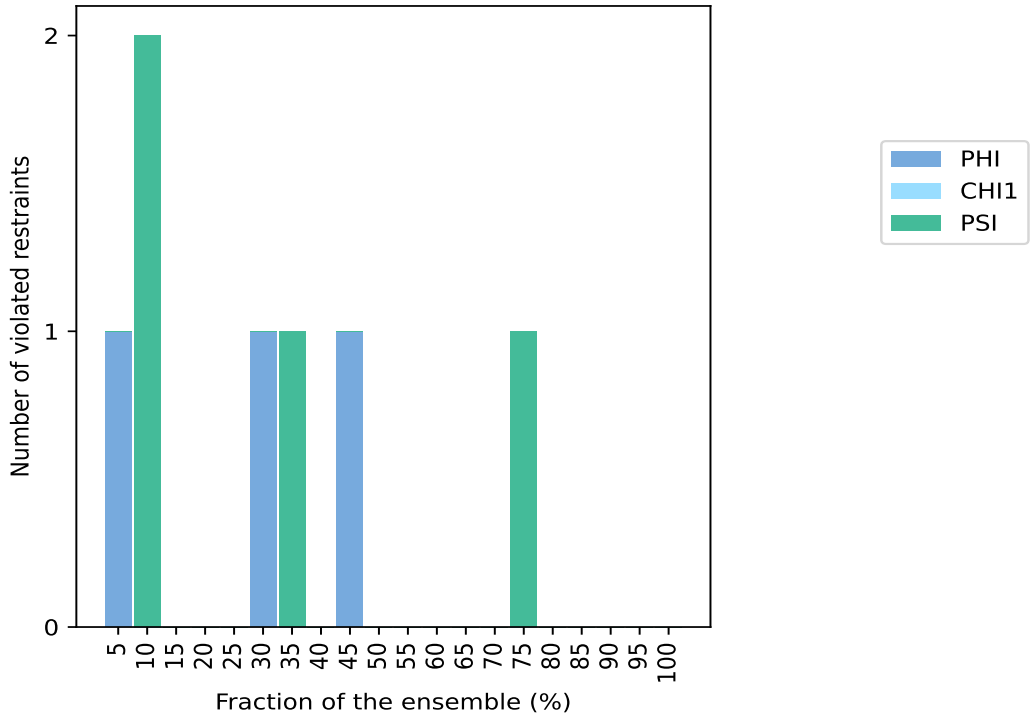
Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	1	1	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

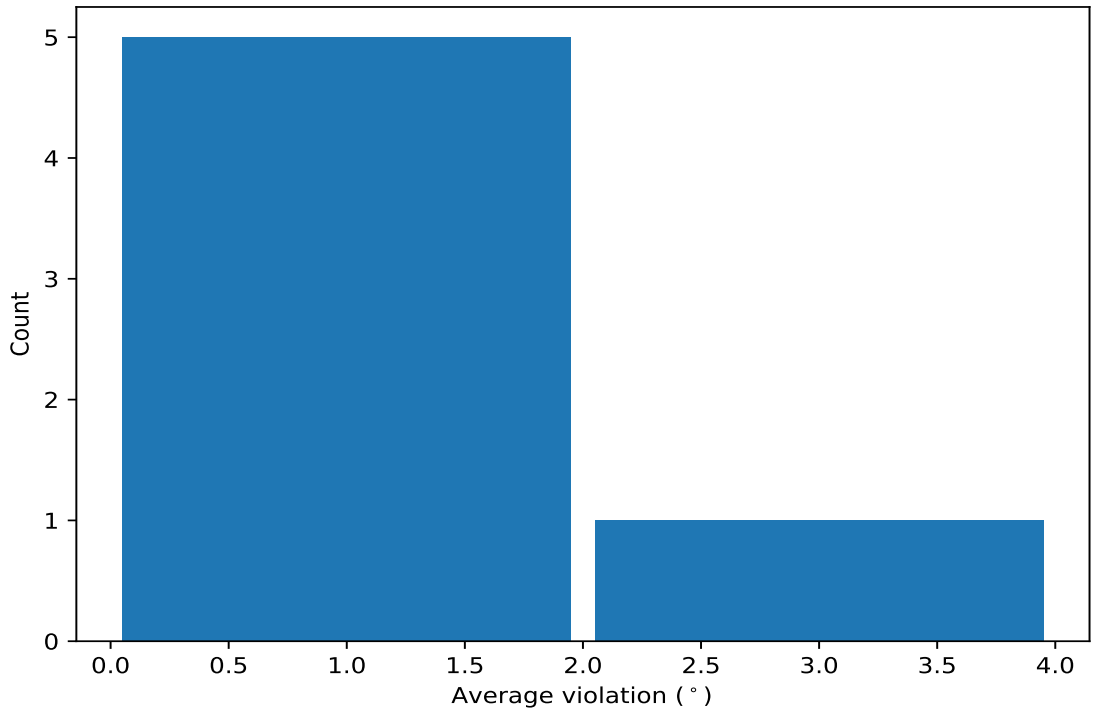


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

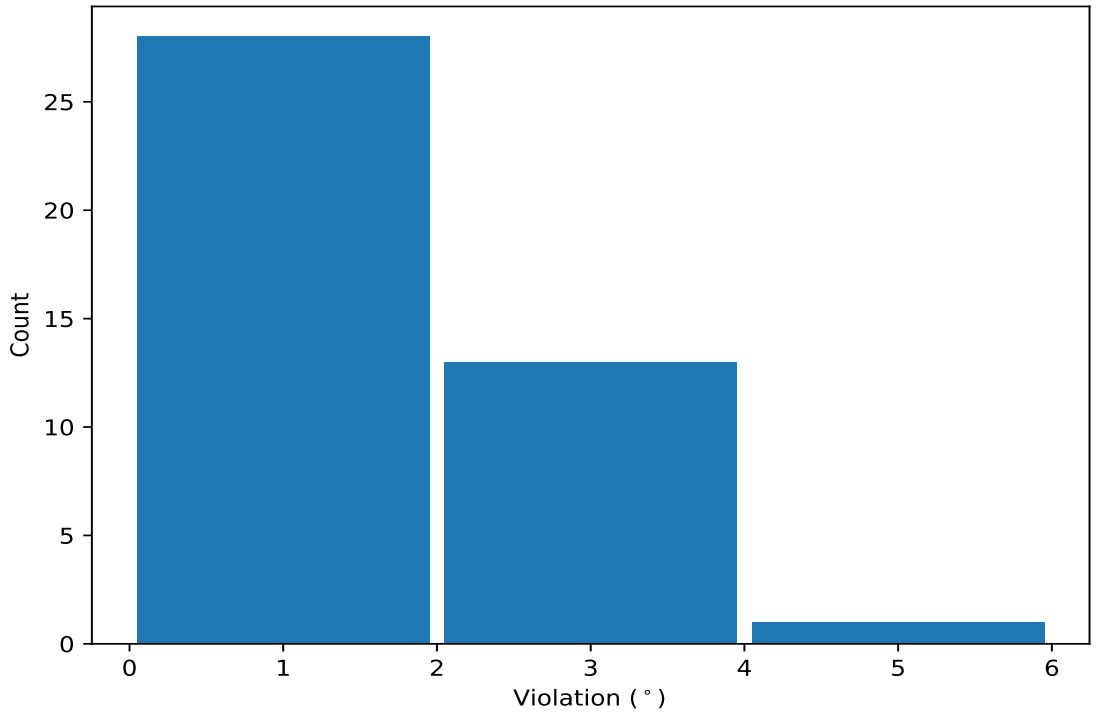
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,42)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:ARG:N	15	1.94	0.62	1.93
(1,14)	1:36:A:MET:C	1:37:A:CYS:N	1:37:A:CYS:CA	1:37:A:CYS:C	9	1.66	0.42	1.63
(1,26)	1:43:A:GLN:N	1:43:A:GLN:CA	1:43:A:GLN:C	1:44:A:ALA:N	7	2.15	1.0	1.74
(1,4)	1:31:A:PRO:C	1:32:A:CYS:N	1:32:A:CYS:CA	1:32:A:CYS:C	6	1.86	0.56	1.74
(1,3)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:CYS:N	2	1.7	0.11	1.7
(1,5)	1:32:A:CYS:N	1:32:A:CYS:CA	1:32:A:CYS:C	1:33:A:GLN:N	2	1.28	0.05	1.28

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:43:A:GLN:N	1:43:A:GLN:CA	1:43:A:GLN:C	1:44:A:ALA:N	17	4.21
(1,42)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:ARG:N	18	3.17
(1,42)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:ARG:N	8	2.99
(1,4)	1:31:A:PRO:C	1:32:A:CYS:N	1:32:A:CYS:CA	1:32:A:CYS:C	5	2.96
(1,26)	1:43:A:GLN:N	1:43:A:GLN:CA	1:43:A:GLN:C	1:44:A:ALA:N	3	2.83
(1,14)	1:36:A:MET:C	1:37:A:CYS:N	1:37:A:CYS:CA	1:37:A:CYS:C	6	2.63
(1,42)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:ARG:N	9	2.54
(1,51)	1:56:A:GLY:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	15	2.31
(1,26)	1:43:A:GLN:N	1:43:A:GLN:CA	1:43:A:GLN:C	1:44:A:ALA:N	19	2.29
(1,42)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:ARG:N	10	2.22