wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LJ6
BMRB ID	:	17283
Title	:	Solution Structure and DNA-binding Properties of the Phosphoesterase Domain of DNA Ligase D
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Deposited on	:	2011-09-06

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:

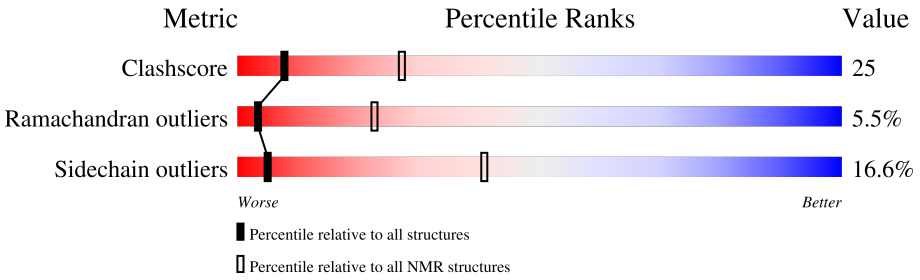
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 69%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	177	29% 32% · 11% 26%

2 Ensemble composition and analysis

This entry contains 15 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:42, A:49-A:93, A:104-A:160 (112)	0.92	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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 7, 9, 15
2	4, 5, 8, 11, 13
3	2, 6, 10, 12
Single-model clusters	14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2075 atoms, of which 1027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable ATP-dependent DNA ligase.

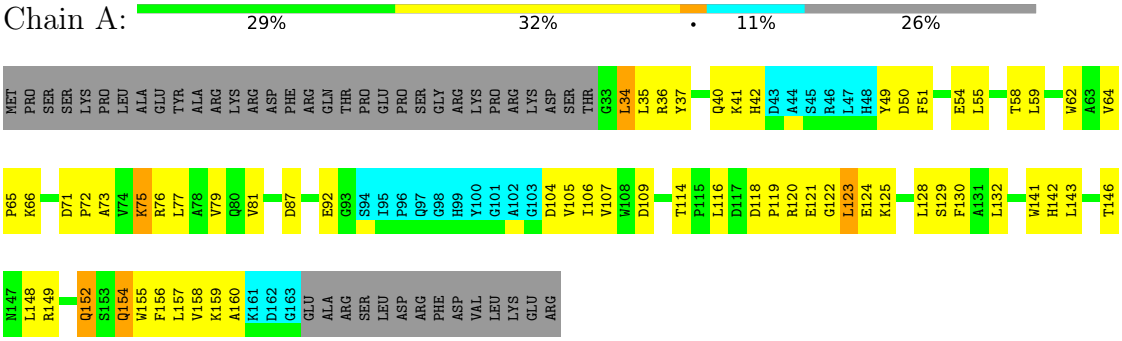
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2075	668	1027	190	188	2	0

4 Residue-property plots

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.

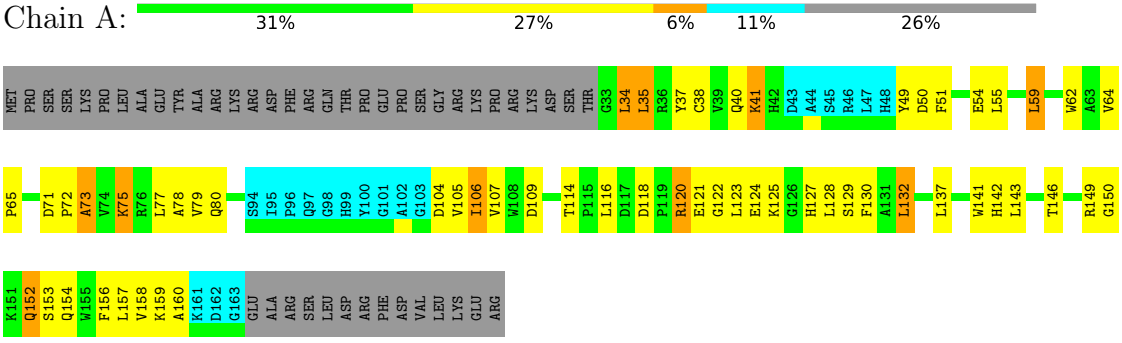
• Molecule 1: Probable ATP-dependent DNA ligase



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: Probable ATP-dependent DNA ligase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 2048 calculated structures, 15 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 solution	2.3
ARIA	refinement	2.3

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	1570
Number of shifts mapped to atoms	1205
Number of unparsed shifts	0
Number of shifts with mapping errors	365
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

6 Model quality

6.1 Standard geometry

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	910	899	894	46±7
All	All	13650	13485	13410	688

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 25.

5 of 344 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:LEU:HD11	1:A:79:VAL:HG23	0.89	1.44	14	2
1:A:64:VAL:HG13	1:A:65:PRO:HA	0.78	1.55	5	4
1:A:146:THR:HG21	1:A:154:GLN:HG3	0.75	1.58	7	3
1:A:41:LYS:CB	1:A:49:TYR:HA	0.73	2.14	13	1
1:A:116:LEU:HD22	1:A:130:PHE:N	0.73	1.98	11	6

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/177 (63%)	87±3 (79±3%)	18±3 (16±3%)	6±2 (5±1%)	3	23
All	All	1665/2655 (63%)	1310 (79%)	264 (16%)	91 (5%)	3	23

5 of 26 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	152	GLN	15
1	A	34	LEU	10
1	A	73	ALA	10
1	A	66	LYS	8
1	A	87	ASP	5

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	95/150 (63%)	79±3 (83±3%)	16±3 (17±3%)	5	41
All	All	1425/2250 (63%)	1188 (83%)	237 (17%)	5	41

5 of 58 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	34	LEU	14
1	A	75	LYS	14
1	A	106	ILE	13
1	A	116	LEU	11
1	A	154	GLN	11

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 69% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1570
Number of shifts mapped to atoms	1205
Number of unparsed shifts	0
Number of shifts with mapping errors	365
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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 365) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	PRO	HA	4.433	0.05	1
1	A	2	PRO	HB2	2.297	0.05	2
1	A	2	PRO	HB3	1.92	0.05	2
1	A	2	PRO	HG2	1.925	0.05	2
1	A	2	PRO	C	176.93	0.11	1
1	A	2	PRO	CA	62.812	0.25	1
1	A	2	PRO	CB	32.495	0.25	1
1	A	2	PRO	CD	51.394	0.30	1
1	A	2	PRO	CG	27.649	0.30	1
1	A	3	SER	H	8.409	0.01	1
1	A	3	SER	HA	4.434	0.05	1
1	A	3	SER	HB2	3.868	0.05	2
1	A	3	SER	C	174.651	0.11	1
1	A	3	SER	CA	58.599	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	SER	CB	63.34	0.25	1
1	A	3	SER	N	115.966	0.14	1
1	A	4	SER	H	8.291	0.01	1
1	A	4	SER	HA	4.458	0.05	1
1	A	4	SER	HB2	3.844	0.05	2
1	A	4	SER	C	174.039	0.11	1
1	A	4	SER	CA	58.522	0.25	1
1	A	4	SER	CB	63.434	0.25	1
1	A	4	SER	N	117.933	0.14	1
1	A	5	LYS	H	8.225	0.01	1
1	A	5	LYS	HB2	1.779	0.05	2
1	A	5	LYS	HD2	1.678	0.05	2
1	A	5	LYS	HG2	1.41	0.05	2
1	A	5	LYS	C	174.433	0.11	1
1	A	5	LYS	CA	54.183	0.25	1
1	A	5	LYS	CB	31.489	0.25	1
1	A	5	LYS	N	124.188	0.14	1
1	A	6	PRO	HA	4.392	0.05	1
1	A	6	PRO	HB2	2.266	0.05	2
1	A	6	PRO	HB3	1.855	0.05	2
1	A	6	PRO	HG2	2.271	0.05	2
1	A	6	PRO	HG3	2.003	0.05	2
1	A	6	PRO	C	177.06	0.11	1
1	A	6	PRO	CA	63.627	0.25	1
1	A	6	PRO	CB	32.595	0.25	1
1	A	6	PRO	CD	51.261	0.30	1
1	A	6	PRO	CG	27.575	0.30	1
1	A	7	LEU	H	8.271	0.01	1
1	A	7	LEU	HA	4.232	0.05	1
1	A	7	LEU	HB2	1.571	0.05	2
1	A	7	LEU	HD11	0.887	0.05	2
1	A	7	LEU	HD12	0.887	0.05	2
1	A	7	LEU	HD13	0.887	0.05	2
1	A	7	LEU	HD21	0.887	0.05	2
1	A	7	LEU	HD22	0.887	0.05	2
1	A	7	LEU	HD23	0.887	0.05	2
1	A	7	LEU	HG	1.599	0.05	1
1	A	7	LEU	C	177.601	0.11	1
1	A	7	LEU	CA	55.738	0.25	1
1	A	7	LEU	CB	42.501	0.25	1
1	A	7	LEU	CD1	24.943	0.30	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	LEU	CD2	23.853	0.30	2
1	A	7	LEU	CG	27.211	0.30	1
1	A	7	LEU	N	122.437	0.14	1
1	A	8	ALA	H	8.227	0.01	1
1	A	8	ALA	HA	4.201	0.05	1
1	A	8	ALA	HB1	1.305	0.05	1
1	A	8	ALA	HB2	1.305	0.05	1
1	A	8	ALA	HB3	1.305	0.05	1
1	A	8	ALA	C	178.01	0.11	1
1	A	8	ALA	CA	53.651	0.25	1
1	A	8	ALA	CB	19.307	0.25	1
1	A	8	ALA	N	124.192	0.14	1
1	A	9	GLU	H	8.278	0.01	1
1	A	9	GLU	HA	4.118	0.05	1
1	A	9	GLU	HB2	1.883	0.05	2
1	A	9	GLU	HG2	2.141	0.05	2
1	A	9	GLU	C	176.658	0.11	1
1	A	9	GLU	CA	57.41	0.25	1
1	A	9	GLU	CB	30.256	0.25	1
1	A	9	GLU	CG	36.379	0.30	1
1	A	9	GLU	N	119.338	0.14	1
1	A	10	TYR	H	7.938	0.01	1
1	A	10	TYR	HA	4.478	0.05	1
1	A	10	TYR	HB2	3.051	0.05	2
1	A	10	TYR	HB3	2.943	0.05	2
1	A	10	TYR	HD1	7.085	0.05	3
1	A	10	TYR	C	175.765	0.11	1
1	A	10	TYR	CA	58.384	0.25	1
1	A	10	TYR	CB	38.542	0.25	1
1	A	10	TYR	N	119.799	0.14	1
1	A	11	ALA	H	7.942	0.01	1
1	A	11	ALA	HA	4.228	0.05	1
1	A	11	ALA	HB1	1.333	0.05	1
1	A	11	ALA	HB2	1.333	0.05	1
1	A	11	ALA	HB3	1.333	0.05	1
1	A	11	ALA	C	177.48	0.11	1
1	A	11	ALA	CA	53.407	0.25	1
1	A	11	ALA	CB	19.326	0.25	1
1	A	11	ALA	N	124.512	0.14	1
1	A	12	ARG	H	7.998	0.01	1
1	A	12	ARG	HA	4.234	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ARG	HB2	1.831	0.05	2
1	A	12	ARG	HB3	1.754	0.05	2
1	A	12	ARG	HD2	3.062	0.05	2
1	A	12	ARG	HG2	1.606	0.05	2
1	A	12	ARG	C	176.639	0.11	1
1	A	12	ARG	CA	56.541	0.25	1
1	A	12	ARG	CB	30.869	0.25	1
1	A	12	ARG	CD	43.544	0.30	1
1	A	12	ARG	CG	27.3	0.30	1
1	A	12	ARG	N	119.719	0.14	1
1	A	13	LYS	H	8.205	0.01	1
1	A	13	LYS	HA	4.233	0.05	1
1	A	13	LYS	HB2	1.771	0.05	2
1	A	13	LYS	HD2	1.814	0.05	2
1	A	13	LYS	HG2	1.414	0.05	2
1	A	13	LYS	C	176.657	0.11	1
1	A	13	LYS	CA	56.868	0.25	1
1	A	13	LYS	CB	32.595	0.25	1
1	A	13	LYS	CD	27.575	0.30	1
1	A	13	LYS	CE	42.356	0.30	1
1	A	13	LYS	CG	24.905	0.30	1
1	A	13	LYS	N	122.321	0.14	1
1	A	14	ARG	H	8.259	0.01	1
1	A	14	ARG	HA	4.218	0.05	1
1	A	14	ARG	HB2	1.691	0.05	2
1	A	14	ARG	HD2	2.912	0.05	2
1	A	14	ARG	HG2	1.701	0.05	2
1	A	14	ARG	HG3	1.523	0.05	2
1	A	14	ARG	C	175.709	0.11	1
1	A	14	ARG	CA	56.475	0.25	1
1	A	14	ARG	CB	30.892	0.25	1
1	A	14	ARG	CD	43.511	0.30	1
1	A	14	ARG	CG	27.062	0.30	1
1	A	14	ARG	N	122.044	0.14	1
1	A	15	ASP	H	8.216	0.01	1
1	A	15	ASP	HA	4.551	0.05	1
1	A	15	ASP	HB2	2.637	0.05	2
1	A	15	ASP	HB3	2.536	0.05	2
1	A	15	ASP	C	175.967	0.11	1
1	A	15	ASP	CA	54.209	0.25	1
1	A	15	ASP	CB	41.436	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	ASP	N	121.138	0.14	1
1	A	16	PHE	H	8.12	0.01	1
1	A	16	PHE	HA	4.547	0.05	1
1	A	16	PHE	HB2	3.131	0.05	2
1	A	16	PHE	HB3	3.029	0.05	2
1	A	16	PHE	HD1	7.221	0.05	3
1	A	16	PHE	C	175.629	0.11	1
1	A	16	PHE	CA	58.239	0.25	1
1	A	16	PHE	CB	39.432	0.25	1
1	A	16	PHE	N	121.184	0.14	1
1	A	17	ARG	H	8.126	0.01	1
1	A	17	ARG	HA	4.213	0.05	1
1	A	17	ARG	HB2	1.721	0.05	2
1	A	17	ARG	HD2	3.002	0.05	2
1	A	17	ARG	HG2	1.506	0.05	2
1	A	17	ARG	C	175.971	0.11	1
1	A	17	ARG	CA	56.384	0.25	1
1	A	17	ARG	CB	30.66	0.25	1
1	A	17	ARG	CD	43.475	0.30	1
1	A	17	ARG	CG	27.155	0.30	1
1	A	17	ARG	N	122.397	0.14	1
1	A	18	GLN	H	8.269	0.01	1
1	A	18	GLN	HA	4.311	0.05	1
1	A	18	GLN	HB2	2.081	0.05	2
1	A	18	GLN	HB3	1.956	0.05	2
1	A	18	GLN	HG2	2.329	0.05	2
1	A	18	GLN	C	175.817	0.11	1
1	A	18	GLN	CA	56.054	0.25	1
1	A	18	GLN	CB	29.655	0.25	1
1	A	18	GLN	CG	34.01	0.30	1
1	A	18	GLN	N	121.24	0.14	1
1	A	19	THR	H	8.183	0.01	1
1	A	19	THR	HA	4.131	0.05	1
1	A	19	THR	HG21	1.212	0.05	1
1	A	19	THR	HG22	1.212	0.05	1
1	A	19	THR	HG23	1.212	0.05	1
1	A	19	THR	C	172.658	0.11	1
1	A	19	THR	CA	59.48	0.25	1
1	A	19	THR	CB	69.156	0.25	1
1	A	19	THR	N	118.156	0.14	1
1	A	20	PRO	HA	4.41	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	PRO	HB2	2.248	0.05	2
1	A	20	PRO	HB3	1.852	0.05	2
1	A	20	PRO	HD2	3.797	0.05	2
1	A	20	PRO	HD3	3.673	0.05	2
1	A	20	PRO	HG2	2.255	0.05	2
1	A	20	PRO	HG3	1.997	0.05	2
1	A	20	PRO	C	176.706	0.11	1
1	A	20	PRO	CA	63.471	0.25	1
1	A	20	PRO	CB	32.299	0.25	1
1	A	20	PRO	CD	51.679	0.30	1
1	A	20	PRO	CG	27.369	0.30	1
1	A	21	GLU	H	8.452	0.01	1
1	A	21	GLU	HA	4.512	0.05	1
1	A	21	GLU	HB2	1.86	0.05	2
1	A	21	GLU	HG2	2.267	0.05	2
1	A	21	GLU	HG3	1.991	0.05	2
1	A	21	GLU	CA	54.02	0.25	1
1	A	21	GLU	CB	28.81	0.25	1
1	A	21	GLU	N	122.764	0.14	1
1	A	22	PRO	HA	4.441	0.05	1
1	A	22	PRO	HB2	2.297	0.05	2
1	A	22	PRO	HB3	1.92	0.05	2
1	A	22	PRO	HG2	2.303	0.05	2
1	A	22	PRO	HG3	2.05	0.05	2
1	A	22	PRO	C	177.232	0.11	1
1	A	22	PRO	CA	63.967	0.25	1
1	A	22	PRO	CB	32.495	0.25	1
1	A	22	PRO	CD	51.394	0.30	1
1	A	22	PRO	CG	27.649	0.30	1
1	A	23	SER	H	8.412	0.01	1
1	A	23	SER	HA	4.394	0.05	1
1	A	23	SER	HB2	3.889	0.05	2
1	A	23	SER	C	175.299	0.11	1
1	A	23	SER	CA	59.052	0.25	1
1	A	23	SER	CB	63.212	0.25	1
1	A	23	SER	N	115.967	0.14	1
1	A	24	GLY	H	8.365	0.01	1
1	A	24	GLY	HA2	3.959	0.05	2
1	A	24	GLY	C	173.979	0.11	1
1	A	24	GLY	CA	45.506	0.25	1
1	A	24	GLY	N	110.63	0.14	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	ARG	H	8.073	0.01	1
1	A	25	ARG	HA	4.315	0.05	1
1	A	25	ARG	HB2	1.798	0.05	2
1	A	25	ARG	HB3	1.699	0.05	2
1	A	25	ARG	HD2	3.164	0.05	2
1	A	25	ARG	HG2	1.585	0.05	2
1	A	25	ARG	C	176.184	0.11	1
1	A	25	ARG	CA	56.24	0.25	1
1	A	25	ARG	CB	30.997	0.25	1
1	A	25	ARG	CD	43.544	0.30	1
1	A	25	ARG	CG	27.243	0.30	1
1	A	25	ARG	N	120.435	0.14	1
1	A	26	LYS	H	8.355	0.01	1
1	A	26	LYS	HA	4.556	0.05	1
1	A	26	LYS	HB2	1.696	0.05	2
1	A	26	LYS	HD2	1.793	0.05	2
1	A	26	LYS	HG2	1.458	0.05	2
1	A	26	LYS	C	174.518	0.11	1
1	A	26	LYS	CA	53.839	0.25	1
1	A	26	LYS	CB	31.381	0.25	1
1	A	26	LYS	N	124.221	0.14	1
1	A	27	PRO	HA	4.393	0.05	1
1	A	27	PRO	HB2	2.261	0.05	2
1	A	27	PRO	HB3	1.843	0.05	2
1	A	27	PRO	HD2	3.795	0.05	2
1	A	27	PRO	HD3	3.61	0.05	2
1	A	27	PRO	HG2	2.271	0.05	2
1	A	27	PRO	HG3	1.99	0.05	2
1	A	27	PRO	C	176.716	0.11	1
1	A	27	PRO	CA	63.449	0.25	1
1	A	27	PRO	CB	32.36	0.25	1
1	A	27	PRO	CD	51.299	0.30	1
1	A	27	PRO	CG	27.49	0.30	1
1	A	28	ARG	H	8.414	0.01	1
1	A	28	ARG	HA	4.29	0.05	1
1	A	28	ARG	HB2	1.821	0.05	2
1	A	28	ARG	HB3	1.755	0.05	2
1	A	28	ARG	HD2	3.186	0.05	2
1	A	28	ARG	HG2	1.632	0.05	2
1	A	28	ARG	C	176.645	0.11	1
1	A	28	ARG	CA	56.347	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	28	ARG	CB	31.392	0.25	1
1	A	28	ARG	CD	43.528	0.30	1
1	A	28	ARG	CG	27.369	0.30	1
1	A	28	ARG	N	121.86	0.14	1
1	A	29	LYS	H	8.443	0.01	1
1	A	29	LYS	HA	4.278	0.05	1
1	A	29	LYS	HB2	1.756	0.05	2
1	A	29	LYS	HD2	1.767	0.05	2
1	A	29	LYS	HG2	1.394	0.05	2
1	A	29	LYS	C	176.192	0.11	1
1	A	29	LYS	CA	56.75	0.25	1
1	A	29	LYS	CB	33.179	0.25	1
1	A	29	LYS	CD	29.139	0.30	1
1	A	29	LYS	CE	42.265	0.30	1
1	A	29	LYS	CG	24.696	0.30	1
1	A	29	LYS	N	123.155	0.14	1
1	A	30	ASP	H	8.356	0.01	1
1	A	30	ASP	HA	4.608	0.05	1
1	A	30	ASP	HB2	2.671	0.05	2
1	A	30	ASP	C	176.315	0.11	1
1	A	30	ASP	CA	54.517	0.25	1
1	A	30	ASP	CB	41.489	0.25	1
1	A	30	ASP	N	121.395	0.14	1
1	A	31	SER	H	8.285	0.01	1
1	A	31	SER	HA	3.876	0.05	1
1	A	31	SER	HB2	4.492	0.05	2
1	A	31	SER	C	174.869	0.11	1
1	A	31	SER	CA	58.645	0.25	1
1	A	31	SER	CB	63.085	0.25	1
1	A	31	SER	N	116.349	0.14	1
1	A	32	THR	H	8.231	0.01	1
1	A	32	THR	HA	4.218	0.05	1
1	A	32	THR	HB	3.892	0.05	1
1	A	32	THR	HG21	1.198	0.05	1
1	A	32	THR	HG22	1.198	0.05	1
1	A	32	THR	HG23	1.198	0.05	1
1	A	32	THR	C	175.264	0.11	1
1	A	32	THR	CA	63.065	0.25	1
1	A	32	THR	CB	70.553	0.25	1
1	A	32	THR	CG2	21.644	0.30	1
1	A	32	THR	N	115.872	0.14	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	ALA	HA	4.409	0.05	1
1	A	165	ALA	HB1	1.49	0.05	1
1	A	165	ALA	HB2	1.49	0.05	1
1	A	165	ALA	HB3	1.49	0.05	1
1	A	165	ALA	C	177.784	0.11	1
1	A	165	ALA	CA	51.93	0.25	1
1	A	165	ALA	CB	19.505	0.25	1
1	A	166	ARG	H	8.159	0.01	1
1	A	166	ARG	HA	4.534	0.05	1
1	A	166	ARG	HB2	1.87	0.05	2
1	A	166	ARG	HG2	1.576	0.05	2
1	A	166	ARG	CA	54.45	0.25	1
1	A	166	ARG	CB	32.69	0.25	1
1	A	166	ARG	N	120.304	0.14	1
1	A	169	ASP	HA	5.45	0.05	1
1	A	169	ASP	HB2	2.881	0.05	2
1	A	169	ASP	C	175.221	0.11	1
1	A	169	ASP	CA	52.512	0.25	1
1	A	169	ASP	CB	43.586	0.25	1
1	A	170	ARG	H	9.098	0.01	1
1	A	170	ARG	CA	56.423	0.25	1
1	A	170	ARG	CB	29.703	0.25	1
1	A	170	ARG	N	124.771	0.14	1
1	A	171	PHE	H	7.642	0.01	1
1	A	171	PHE	HD1	7.101	0.05	3
1	A	171	PHE	C	180.394	0.11	1
1	A	171	PHE	CA	58.603	0.25	1
1	A	171	PHE	CB	38.66	0.25	1
1	A	171	PHE	N	124.753	0.14	1
1	A	172	ASP	H	8.543	0.01	1
1	A	173	VAL	C	176.523	0.11	1
1	A	174	LEU	H	8.383	0.01	1
1	A	174	LEU	N	122.289	0.14	1
1	A	175	LYS	HA	4.398	0.05	1
1	A	175	LYS	HB2	1.855	0.05	2
1	A	175	LYS	HB3	1.73	0.05	2
1	A	175	LYS	HD2	1.741	0.05	2
1	A	175	LYS	HE2	3.092	0.05	2
1	A	175	LYS	HG2	1.364	0.05	2
1	A	175	LYS	C	176.697	0.11	1
1	A	175	LYS	CA	56.759	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	175	LYS	CB	32.569	0.25	1
1	A	175	LYS	CD	29.281	0.30	1
1	A	175	LYS	CE	43.533	0.30	1
1	A	175	LYS	CG	25.127	0.30	1
1	A	176	GLU	H	8.14	0.01	1
1	A	176	GLU	HA	4.302	0.05	1
1	A	176	GLU	HB2	2.127	0.05	2
1	A	176	GLU	HB3	1.836	0.05	2
1	A	176	GLU	HG2	2.241	0.05	2
1	A	176	GLU	C	175.684	0.11	1
1	A	176	GLU	CA	57.025	0.25	1
1	A	176	GLU	CB	30.765	0.25	1
1	A	176	GLU	CG	36.463	0.30	1
1	A	176	GLU	N	121.697	0.14	1
1	A	177	ARG	H	7.959	0.01	1
1	A	177	ARG	HA	4.228	0.05	1
1	A	177	ARG	HB2	1.782	0.05	2
1	A	177	ARG	HD2	3.235	0.05	2
1	A	177	ARG	HG2	1.644	0.05	2
1	A	177	ARG	C	181.008	0.11	1
1	A	177	ARG	CA	56.798	0.25	1
1	A	177	ARG	CB	30.461	0.25	1
1	A	177	ARG	N	126.421	0.14	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	164	-0.19 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	150	0.13 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	157	0.18 ± 0.12	None needed (< 0.5 ppm)
^{15}N	146	-0.52 ± 0.19	Should be applied

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 69%, i.e. 1086 atoms were assigned a chemical shift out of a possible 1578. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	533/558 (96%)	212/228 (93%)	220/224 (98%)	101/106 (95%)
Sidechain	524/861 (61%)	351/557 (63%)	171/267 (64%)	2/37 (5%)
Aromatic	29/159 (18%)	27/78 (35%)	0/68 (0%)	2/13 (15%)
Overall	1086/1578 (69%)	590/863 (68%)	391/559 (70%)	105/156 (67%)

7.1.4 Statistically unusual chemical shifts (i)

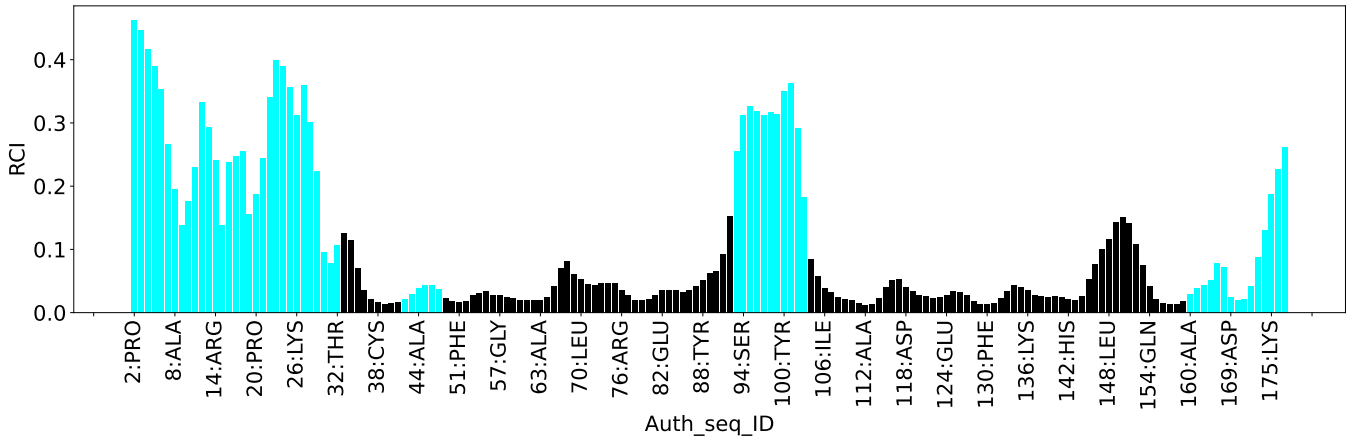
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	53	LEU	HD11	-0.85	-0.61 – 2.12	-5.9
1	A	53	LEU	HD12	-0.85	-0.61 – 2.12	-5.9
1	A	53	LEU	HD13	-0.85	-0.61 – 2.12	-5.9
1	A	143	LEU	HD21	-0.72	-0.65 – 2.13	-5.2
1	A	143	LEU	HD22	-0.72	-0.65 – 2.13	-5.2
1	A	143	LEU	HD23	-0.72	-0.65 – 2.13	-5.2

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	2080
Intra-residue (|i-j|=0)	734
Sequential (|i-j|=1)	546
Medium range (|i-j|>1 and |i-j|<5)	225
Long range (|i-j|≥5)	575
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	458
Number of restraints per residue	11.8
Number of long range restraints per residue[1]	3.2

[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)	52.6	0.2
0.2-0.5 (Medium)	82.5	0.5
>0.5 (Large)	167.9	6.54

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 (i)

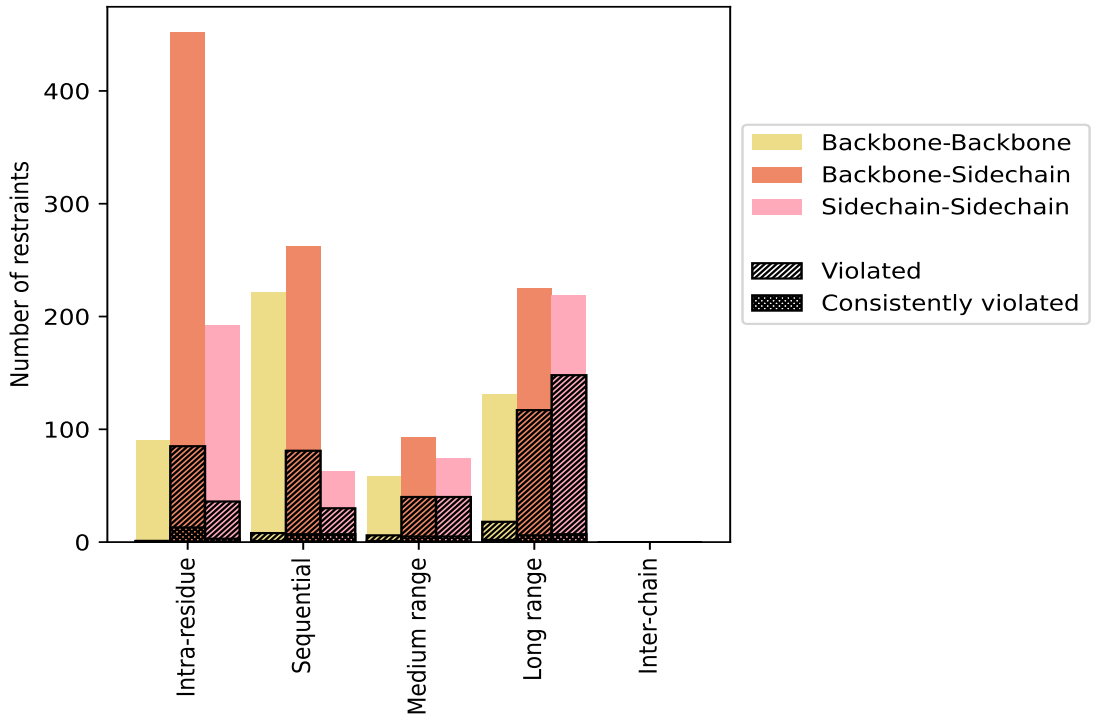
9.1 Summary of distance violations (i)

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)	734	35.3	122	16.6	5.9	17	2.3	0.8
Backbone-Backbone	90	4.3	1	1.1	0.0	1	1.1	0.0
Backbone-Sidechain	452	21.7	85	18.8	4.1	13	2.9	0.6
Sidechain-Sidechain	192	9.2	36	18.8	1.7	3	1.6	0.1
Sequential (|i-j|=1)	546	26.2	119	21.8	5.7	15	2.7	0.7
Backbone-Backbone	221	10.6	8	3.6	0.4	1	0.5	0.0
Backbone-Sidechain	262	12.6	81	30.9	3.9	7	2.7	0.3
Sidechain-Sidechain	63	3.0	30	47.6	1.4	7	11.1	0.3
Medium range (|i-j|>1 & |i-j|<5)	225	10.8	86	38.2	4.1	11	4.9	0.5
Backbone-Backbone	58	2.8	6	10.3	0.3	1	1.7	0.0
Backbone-Sidechain	93	4.5	40	43.0	1.9	5	5.4	0.2
Sidechain-Sidechain	74	3.6	40	54.1	1.9	5	6.8	0.2
Long range (|i-j|≥5)	575	27.6	283	49.2	13.6	15	2.6	0.7
Backbone-Backbone	131	6.3	18	13.7	0.9	2	1.5	0.1
Backbone-Sidechain	225	10.8	117	52.0	5.6	6	2.7	0.3
Sidechain-Sidechain	219	10.5	148	67.6	7.1	7	3.2	0.3
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	2080	100.0	610	29.3	29.3	58	2.8	2.8
Backbone-Backbone	500	24.0	33	6.6	1.6	5	1.0	0.2
Backbone-Sidechain	1032	49.6	323	31.3	15.5	31	3.0	1.5
Sidechain-Sidechain	548	26.3	254	46.4	12.2	22	4.0	1.1

[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	62	52	49	122	0	285	0.91	4.21	0.79	0.68
2	68	56	47	131	0	302	0.88	6.54	0.92	0.53
3	59	56	45	127	0	287	0.86	3.67	0.77	0.64
4	61	58	49	128	0	296	0.84	3.67	0.75	0.54
5	60	59	49	156	0	324	0.94	4.35	0.86	0.64
6	63	56	45	144	0	308	0.93	5.42	0.87	0.64
7	57	54	51	129	0	291	0.75	4.33	0.66	0.52
8	64	55	51	142	0	312	1.0	4.61	0.97	0.68
9	67	53	52	139	0	311	0.84	4.17	0.79	0.55
10	64	64	55	145	0	328	0.92	4.79	0.86	0.68
11	61	52	52	129	0	294	0.87	6.53	0.84	0.58

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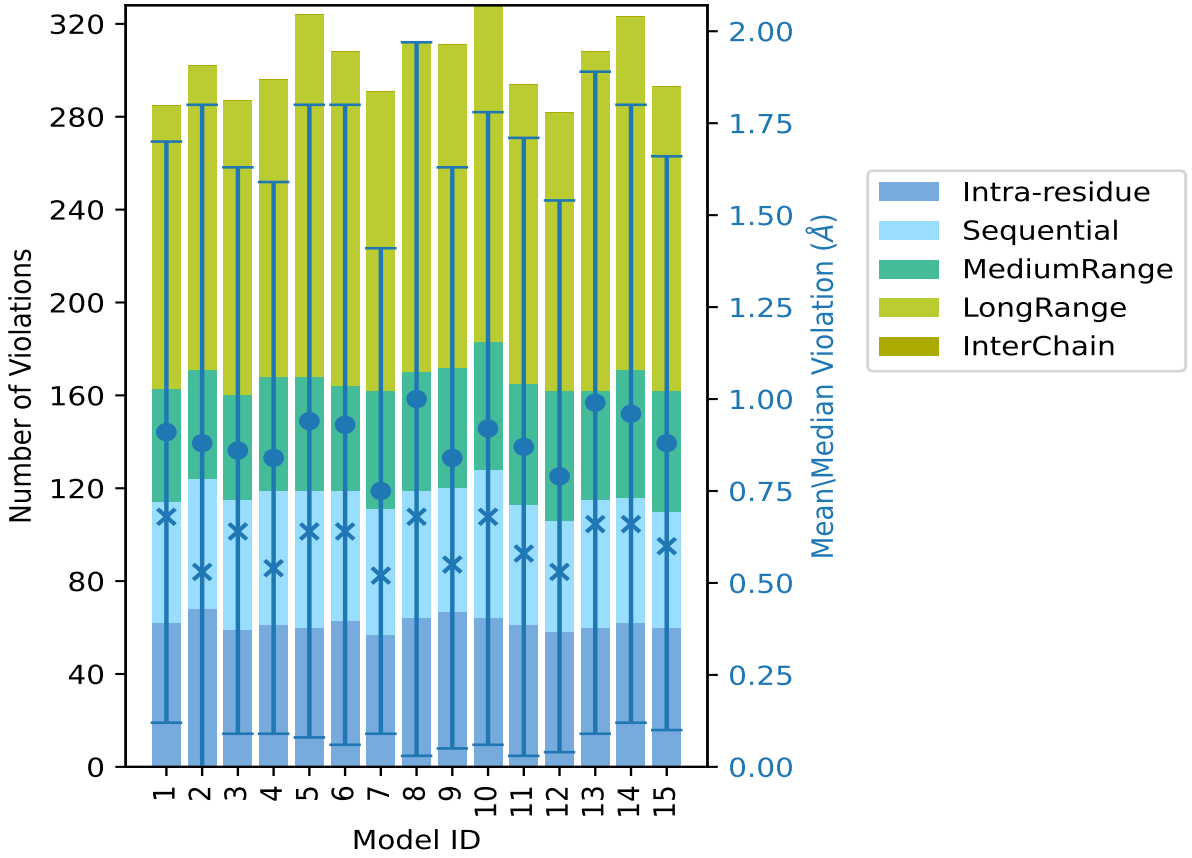
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	58	48	56	120	0	282	0.79	3.84	0.75	0.53
13	60	55	47	146	0	308	0.99	4.87	0.9	0.66
14	62	54	55	152	0	323	0.96	4.18	0.84	0.66
15	60	50	52	131	0	293	0.88	4.06	0.78	0.6

[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

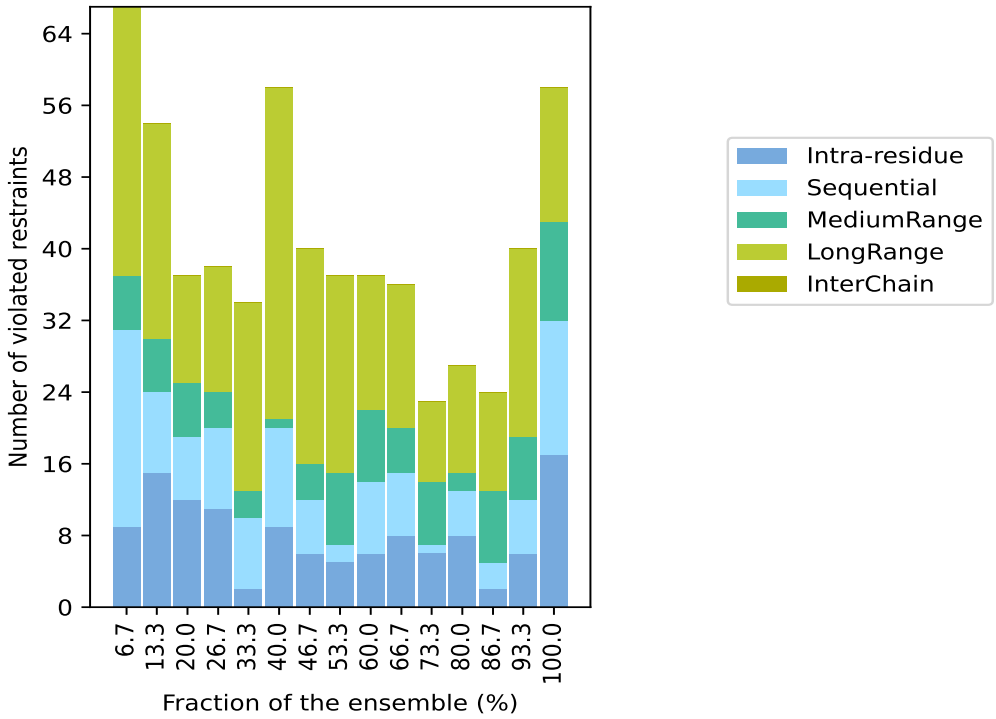
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 1470(IR:612, SQ:427, MR:139, LR:292, 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]	%
9	22	6	30	0	67	1	6.7
15	9	6	24	0	54	2	13.3
12	7	6	12	0	37	3	20.0
11	9	4	14	0	38	4	26.7
2	8	3	21	0	34	5	33.3
9	11	1	37	0	58	6	40.0
6	6	4	24	0	40	7	46.7
5	2	8	22	0	37	8	53.3
6	8	8	15	0	37	9	60.0
8	7	5	16	0	36	10	66.7
6	1	7	9	0	23	11	73.3
8	5	2	12	0	27	12	80.0
2	3	8	11	0	24	13	86.7
6	6	7	21	0	40	14	93.3
17	15	11	15	0	58	15	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

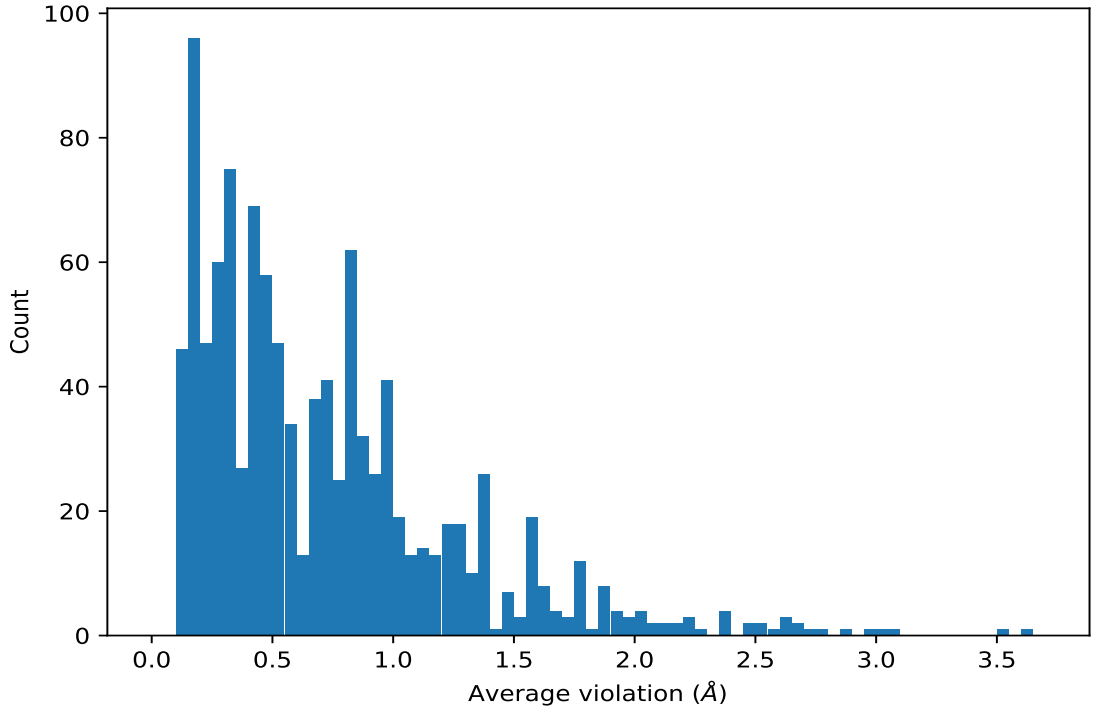
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,204)	1:A:71:ASP:HB2	1:A:74:VAL:HG11	15	3.06	0.96	3.37
(1,312)	1:A:119:PRO:HG3	1:A:120:ARG:HB3	15	2.48	0.57	2.15
(1,525)	1:A:79:VAL:HB	1:A:81:VAL:HG12	15	2.4	0.61	2.56
(1,525)	1:A:79:VAL:HB	1:A:81:VAL:HG11	15	2.4	0.61	2.56
(1,525)	1:A:79:VAL:HB	1:A:81:VAL:HG13	15	2.4	0.61	2.56
(1,300)	1:A:54:GLU:HB3	1:A:59:LEU:HB3	15	2.2	0.99	2.07
(1,1691)	1:A:129:SER:HB2	1:A:115:PRO:HB2	15	1.98	0.7	1.69
(1,498)	1:A:131:ALA:HB1	1:A:114:THR:HG21	15	1.79	0.09	1.82
(1,26)	1:A:115:PRO:HA	1:A:119:PRO:HD2	15	1.76	0.05	1.77
(1,653)	1:A:53:LEU:HD21	1:A:143:LEU:HB3	15	1.7	1.04	1.19
(1,521)	1:A:158:VAL:HG12	1:A:143:LEU:HD12	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG12	1:A:143:LEU:HD11	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG12	1:A:143:LEU:HD13	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG11	1:A:143:LEU:HD12	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG11	1:A:143:LEU:HD11	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG11	1:A:143:LEU:HD13	15	1.59	0.98	1.84

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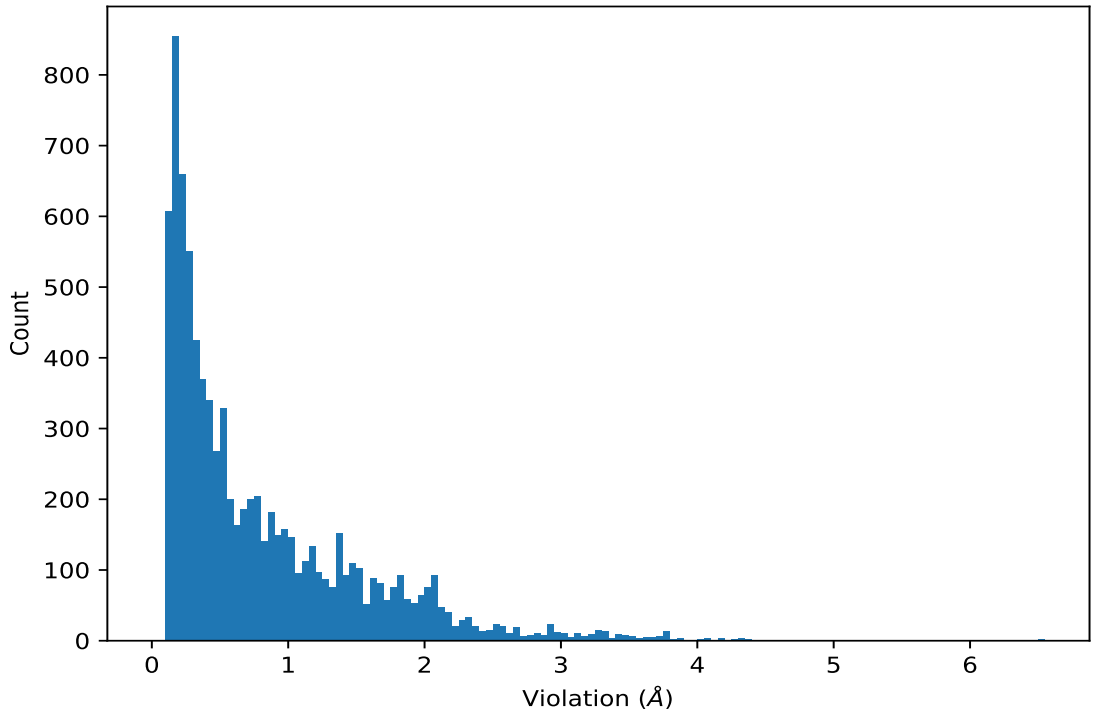
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,521)	1:A:158:VAL:HG13	1:A:143:LEU:HD12	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG13	1:A:143:LEU:HD11	15	1.59	0.98	1.84
(1,521)	1:A:158:VAL:HG13	1:A:143:LEU:HD13	15	1.59	0.98	1.84
(1,514)	1:A:79:VAL:HG11	1:A:77:LEU:HG	15	1.55	1.68	0.28

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(1,445)	1:A:35:LEU:HD11	1:A:55:LEU:HD11	2	6.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:A:35:LEU:HD11	1:A:55:LEU:HD11	11	6.53
(1,464)	1:A:39:VAL:HG11	1:A:49:TYR:HD1	2	6.41
(1,464)	1:A:39:VAL:HG11	1:A:49:TYR:HD1	6	5.42
(1,445)	1:A:35:LEU:HD11	1:A:55:LEU:HD11	13	4.87
(1,427)	1:A:132:LEU:HD21	1:A:51:PHE:HE1	6	4.84
(1,427)	1:A:132:LEU:HD21	1:A:51:PHE:HE1	10	4.79
(1,441)	1:A:39:VAL:HG11	1:A:41:LYS:HB3	8	4.61
(1,464)	1:A:39:VAL:HG11	1:A:49:TYR:HD1	10	4.45
(1,514)	1:A:79:VAL:HG11	1:A:77:LEU:HG	8	4.35

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found