wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2JQQ
BMRB ID	:	15290
Title	:	Solution structure of Saccharomyces cerevisiae conserved oligomeric Golgi subunit 2 protein (Cog2p)
Authors	:	Cavanaugh, L.F.; Chen, X.; Pelczer, I.; Rizo, J.; Hughson, F.M.
Deposited on	:	2007-06-06

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 (1)) were used in the production of this report:

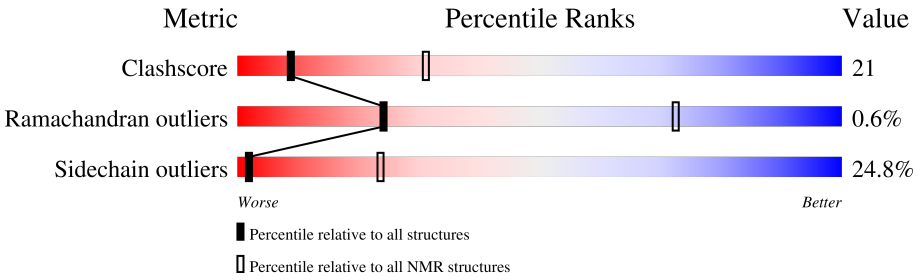
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 93%.

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	204	38% 25% • 9% 25%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:110-A:153, A:158-A:207, A:217-A:258 (136)	0.61	4

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2509 atoms, of which 1272 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Conserved oligomeric Golgi complex subunit 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2509	777	1272	207	247	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	cloning artifact	UNP P53271
A	60	SER	-	cloning artifact	UNP P53271

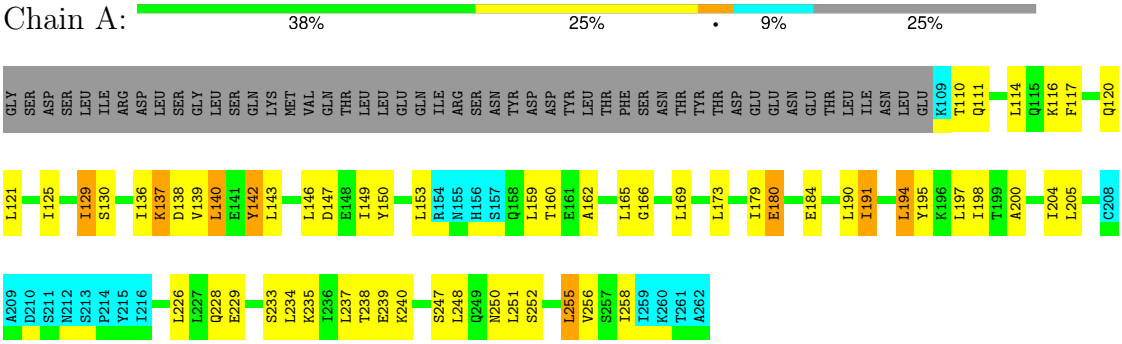
4 Residue-property plots

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: Conserved oligomeric Golgi complex subunit 2

Chain A:

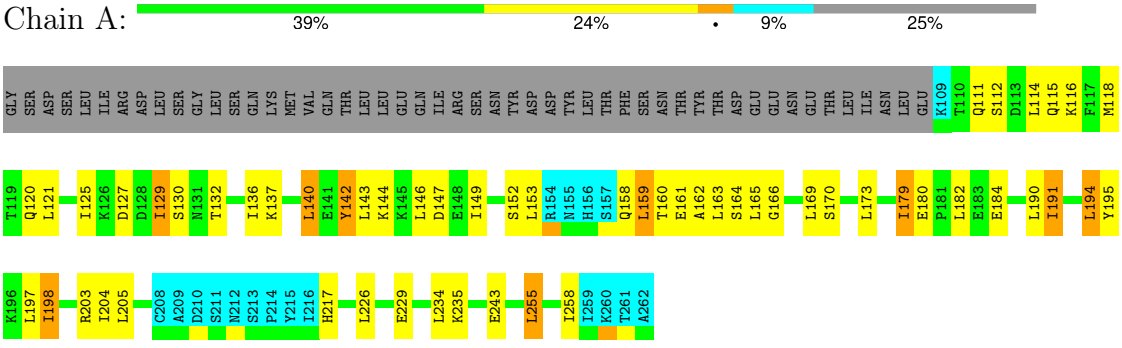


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Conserved oligomeric Golgi complex subunit 2

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 1200 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
CNS	structure solution	1.1
CNS	refinement	1.1
AQUA	refinement	
TALOS	geometry optimization	
ProcheckNMR	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	2446
Number of shifts mapped to atoms	1954
Number of unparsed shifts	0
Number of shifts with mapping errors	492
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	1097	1134	1130	46±6
All	All	21940	22680	22600	916

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 21.

5 of 265 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:VAL:HG11	1:A:190:LEU:HD11	1.08	1.25	12	16
1:A:149:ILE:HG22	1:A:153:LEU:HD12	1.05	1.27	7	13
1:A:162:ALA:HB1	1:A:197:LEU:HD11	1.05	1.23	20	5
1:A:149:ILE:HG21	1:A:162:ALA:HB2	1.02	1.27	12	15
1:A:139:VAL:HG11	1:A:190:LEU:HD21	0.98	1.33	5	2

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	136/204 (67%)	128±2 (94±1%)	7±2 (5±1%)	1±1 (1±1%)	24 72
All	All	2720/4080 (67%)	2566 (94%)	138 (5%)	16 (1%)	24 72

All 5 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	180	GLU	8
1	A	179	ILE	4
1	A	248	LEU	2
1	A	130	SER	1
1	A	153	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	130/194 (67%)	98±4 (75±3%)	32±4 (25±3%)	2 24
All	All	2600/3880 (67%)	1954 (75%)	646 (25%)	2 24

5 of 94 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	116	LYS	20
1	A	140	LEU	20
1	A	142	TYR	20
1	A	191	ILE	20
1	A	205	LEU	20

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)

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 93% for the well-defined parts and 90% 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	2446
Number of shifts mapped to atoms	1954
Number of unparsed shifts	0
Number of shifts with mapping errors	492
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 492) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	ASP	H	8.53	0.03	1
1	A	61	ASP	HA	4.62	0.03	1
1	A	61	ASP	HB2	2.68	0.03	2
1	A	61	ASP	HB3	2.68	0.03	2
1	A	61	ASP	C	174.49	0.3	1
1	A	61	ASP	CA	55.04	0.3	1
1	A	61	ASP	CB	41.5	0.3	1
1	A	61	ASP	N	122.14	0.3	1
1	A	62	SER	H	8.13	0.03	1
1	A	62	SER	HA	4.38	0.03	1
1	A	62	SER	HB2	3.85	0.03	2
1	A	62	SER	HB3	3.85	0.03	2
1	A	62	SER	C	176.51	0.3	1
1	A	62	SER	CA	59.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	SER	CB	64.2	0.3	1
1	A	62	SER	N	115.49	0.3	1
1	A	63	LEU	H	8.16	0.03	1
1	A	63	LEU	HA	4.3	0.03	1
1	A	63	LEU	HB2	1.59	0.03	2
1	A	63	LEU	HB3	1.66	0.03	2
1	A	63	LEU	HD11	0.9	0.03	2
1	A	63	LEU	HD12	0.9	0.03	2
1	A	63	LEU	HD13	0.9	0.03	2
1	A	63	LEU	HD21	0.85	0.03	2
1	A	63	LEU	HD22	0.85	0.03	2
1	A	63	LEU	HD23	0.85	0.03	2
1	A	63	LEU	HG	1.61	0.03	1
1	A	63	LEU	C	174.65	0.3	1
1	A	63	LEU	CA	56.2	0.3	1
1	A	63	LEU	CB	42.7	0.3	1
1	A	63	LEU	CD1	25.4	0.3	1
1	A	63	LEU	CD2	24.3	0.3	1
1	A	63	LEU	CG	27.7	0.3	1
1	A	63	LEU	N	123.75	0.3	1
1	A	64	ILE	H	7.93	0.03	1
1	A	64	ILE	HA	4.07	0.03	1
1	A	64	ILE	HB	1.85	0.03	1
1	A	64	ILE	HD11	0.83	0.03	1
1	A	64	ILE	HD12	0.83	0.03	1
1	A	64	ILE	HD13	0.83	0.03	1
1	A	64	ILE	HG12	1.17	0.03	1
1	A	64	ILE	HG13	1.46	0.03	1
1	A	64	ILE	HG21	0.85	0.03	1
1	A	64	ILE	HG22	0.85	0.03	1
1	A	64	ILE	HG23	0.85	0.03	1
1	A	64	ILE	C	177.38	0.3	1
1	A	64	ILE	CA	61.9	0.3	1
1	A	64	ILE	CB	38.7	0.3	1
1	A	64	ILE	CD1	13.3	0.3	1
1	A	64	ILE	CG1	27.8	0.3	1
1	A	64	ILE	CG2	17.8	0.3	1
1	A	64	ILE	N	119.86	0.3	1
1	A	65	ARG	H	8.14	0.03	1
1	A	65	ARG	HA	4.25	0.03	1
1	A	65	ARG	HB2	1.74	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	ARG	HB3	1.8	0.03	2
1	A	65	ARG	HD2	3.16	0.03	2
1	A	65	ARG	HD3	3.16	0.03	2
1	A	65	ARG	HG2	1.61	0.03	2
1	A	65	ARG	HG3	1.57	0.03	2
1	A	65	ARG	C	176.36	0.3	1
1	A	65	ARG	CA	56.9	0.3	1
1	A	65	ARG	CB	31.2	0.3	1
1	A	65	ARG	CD	43.6	0.3	1
1	A	65	ARG	CG	27.5	0.3	1
1	A	65	ARG	N	124.19	0.3	1
1	A	66	ASP	H	8.18	0.03	1
1	A	66	ASP	HA	4.6	0.03	1
1	A	66	ASP	HB2	2.65	0.03	2
1	A	66	ASP	HB3	2.75	0.03	2
1	A	66	ASP	C	175.94	0.3	1
1	A	66	ASP	CA	54.9	0.3	1
1	A	66	ASP	CB	41.5	0.3	1
1	A	66	ASP	N	120.77	0.3	1
1	A	67	LEU	H	8.35	0.03	1
1	A	67	LEU	HA	4.31	0.03	1
1	A	67	LEU	HB2	1.66	0.03	2
1	A	67	LEU	HB3	1.66	0.03	2
1	A	67	LEU	HD11	0.82	0.03	2
1	A	67	LEU	HD12	0.82	0.03	2
1	A	67	LEU	HD13	0.82	0.03	2
1	A	67	LEU	HD21	0.79	0.03	2
1	A	67	LEU	HD22	0.79	0.03	2
1	A	67	LEU	HD23	0.79	0.03	2
1	A	67	LEU	HG	1.65	0.03	1
1	A	67	LEU	C	176.76	0.3	1
1	A	67	LEU	CA	56.0	0.3	1
1	A	67	LEU	CB	42.1	0.3	1
1	A	67	LEU	CD1	26.0	0.3	1
1	A	67	LEU	CD2	23.7	0.3	1
1	A	67	LEU	CG	27.3	0.3	1
1	A	67	LEU	N	123.85	0.3	1
1	A	68	SER	H	8.25	0.03	1
1	A	68	SER	HA	4.22	0.03	1
1	A	68	SER	HB2	3.91	0.03	2
1	A	68	SER	HB3	3.91	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	SER	C	177.84	0.3	1
1	A	68	SER	CA	60.6	0.3	1
1	A	68	SER	CB	63.9	0.3	1
1	A	68	SER	N	115.34	0.3	1
1	A	69	GLY	H	8.25	0.03	1
1	A	69	GLY	HA2	4.01	0.03	2
1	A	69	GLY	HA3	3.83	0.03	2
1	A	69	GLY	C	175.37	0.3	1
1	A	69	GLY	CA	45.8	0.3	1
1	A	69	GLY	N	109.85	0.3	1
1	A	70	LEU	H	7.68	0.03	1
1	A	70	LEU	HA	4.38	0.03	1
1	A	70	LEU	HB2	1.67	0.03	2
1	A	70	LEU	HB3	1.45	0.03	2
1	A	70	LEU	HD11	0.81	0.03	2
1	A	70	LEU	HD12	0.81	0.03	2
1	A	70	LEU	HD13	0.81	0.03	2
1	A	70	LEU	HD21	0.83	0.03	2
1	A	70	LEU	HD22	0.83	0.03	2
1	A	70	LEU	HD23	0.83	0.03	2
1	A	70	LEU	HG	1.66	0.03	1
1	A	70	LEU	C	174.62	0.3	1
1	A	70	LEU	CA	55.6	0.3	1
1	A	70	LEU	CB	43.1	0.3	1
1	A	70	LEU	CD1	24.3	0.3	1
1	A	70	LEU	CD2	26.0	0.3	1
1	A	70	LEU	CG	27.3	0.3	1
1	A	70	LEU	N	121.55	0.3	1
1	A	71	SER	H	8.06	0.03	1
1	A	71	SER	CB	65.16	0.3	1
1	A	71	SER	N	118.09	0.3	1
1	A	73	LYS	H	8.17	0.03	1
1	A	73	LYS	HA	4.12	0.03	1
1	A	73	LYS	HB2	1.78	0.03	2
1	A	73	LYS	HB3	1.84	0.03	2
1	A	73	LYS	HD2	1.71	0.03	2
1	A	73	LYS	HD3	1.71	0.03	2
1	A	73	LYS	HE2	2.96	0.03	2
1	A	73	LYS	HE3	2.96	0.03	2
1	A	73	LYS	HG2	1.44	0.03	2
1	A	73	LYS	HG3	1.44	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	73	LYS	C	178.44	0.3	1
1	A	73	LYS	CA	59.1	0.3	1
1	A	73	LYS	CB	32.5	0.3	1
1	A	73	LYS	CD	29.3	0.3	1
1	A	73	LYS	CE	41.7	0.3	1
1	A	73	LYS	CG	25.3	0.3	1
1	A	73	LYS	N	118.56	0.3	1
1	A	74	MET	H	7.82	0.03	1
1	A	74	MET	HE1	2.11	0.03	1
1	A	74	MET	HE2	2.11	0.03	1
1	A	74	MET	HE3	2.11	0.03	1
1	A	74	MET	C	179.05	0.3	1
1	A	74	MET	CE	17.5	0.3	1
1	A	74	MET	N	120.4	0.3	1
1	A	75	VAL	H	8.11	0.03	1
1	A	75	VAL	HA	3.47	0.03	1
1	A	75	VAL	HB	2.2	0.03	1
1	A	75	VAL	HG11	0.88	0.03	2
1	A	75	VAL	HG12	0.88	0.03	2
1	A	75	VAL	HG13	0.88	0.03	2
1	A	75	VAL	HG21	0.98	0.03	2
1	A	75	VAL	HG22	0.98	0.03	2
1	A	75	VAL	HG23	0.98	0.03	2
1	A	75	VAL	CA	68.0	0.3	1
1	A	75	VAL	CB	32.2	0.3	1
1	A	75	VAL	CG1	21.7	0.3	1
1	A	75	VAL	CG2	24.2	0.3	1
1	A	75	VAL	N	119.03	0.3	1
1	A	76	GLN	H	8.1	0.03	1
1	A	76	GLN	HA	3.84	0.03	1
1	A	76	GLN	HB2	2.18	0.03	2
1	A	76	GLN	HB3	2.18	0.03	2
1	A	76	GLN	HE21	7.57	0.03	2
1	A	76	GLN	HE22	6.64	0.03	2
1	A	76	GLN	HG2	2.37	0.03	2
1	A	76	GLN	HG3	2.37	0.03	2
1	A	76	GLN	C	177.32	0.3	1
1	A	76	GLN	CA	60.0	0.3	1
1	A	76	GLN	CB	28.6	0.3	1
1	A	76	GLN	CG	34.1	0.3	1
1	A	76	GLN	N	118.12	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	GLN	NE2	111.38	0.3	1
1	A	77	THR	H	7.97	0.03	1
1	A	77	THR	HA	4.34	0.03	1
1	A	77	THR	HB	3.94	0.03	1
1	A	77	THR	HG21	1.24	0.03	1
1	A	77	THR	HG22	1.24	0.03	1
1	A	77	THR	HG23	1.24	0.03	1
1	A	77	THR	CA	67.1	0.3	1
1	A	77	THR	CB	69.4	0.3	1
1	A	77	THR	CG2	21.9	0.3	1
1	A	77	THR	N	115.28	0.3	1
1	A	78	LEU	H	8.04	0.03	1
1	A	78	LEU	HA	4.06	0.03	1
1	A	78	LEU	HB2	1.98	0.03	2
1	A	78	LEU	HB3	1.37	0.03	2
1	A	78	LEU	HD11	0.78	0.03	2
1	A	78	LEU	HD12	0.78	0.03	2
1	A	78	LEU	HD13	0.78	0.03	2
1	A	78	LEU	HD21	0.83	0.03	2
1	A	78	LEU	HD22	0.83	0.03	2
1	A	78	LEU	HD23	0.83	0.03	2
1	A	78	LEU	HG	1.8	0.03	1
1	A	78	LEU	C	176.75	0.3	1
1	A	78	LEU	CA	58.6	0.3	1
1	A	78	LEU	CB	42.3	0.3	1
1	A	78	LEU	CD1	24.2	0.3	1
1	A	78	LEU	CD2	23.1	0.3	1
1	A	78	LEU	CG	27.3	0.3	1
1	A	78	LEU	N	123.02	0.3	1
1	A	79	LEU	H	8.36	0.03	1
1	A	79	LEU	HA	3.96	0.03	1
1	A	79	LEU	HB2	1.99	0.03	2
1	A	79	LEU	HB3	1.99	0.03	2
1	A	79	LEU	HD11	0.87	0.03	2
1	A	79	LEU	HD12	0.87	0.03	2
1	A	79	LEU	HD13	0.87	0.03	2
1	A	79	LEU	HD21	0.91	0.03	2
1	A	79	LEU	HD22	0.91	0.03	2
1	A	79	LEU	HD23	0.91	0.03	2
1	A	79	LEU	HG	1.32	0.03	1
1	A	79	LEU	CA	58.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	LEU	CB	42.1	0.3	1
1	A	79	LEU	CD1	24.2	0.3	1
1	A	79	LEU	CD2	26.5	0.3	1
1	A	79	LEU	CG	26.2	0.3	1
1	A	79	LEU	N	119.51	0.3	1
1	A	80	GLU	H	8.21	0.03	1
1	A	80	GLU	C	178.93	0.3	1
1	A	80	GLU	N	118.33	0.3	1
1	A	81	GLN	H	7.84	0.03	1
1	A	81	GLN	HA	4.01	0.03	1
1	A	81	GLN	HB2	2.24	0.03	2
1	A	81	GLN	HB3	2.19	0.03	2
1	A	81	GLN	HE21	7.24	0.03	2
1	A	81	GLN	HE22	6.73	0.03	2
1	A	81	GLN	HG2	2.33	0.03	2
1	A	81	GLN	HG3	2.5	0.03	2
1	A	81	GLN	CA	59.0	0.3	1
1	A	81	GLN	CB	28.6	0.3	1
1	A	81	GLN	CG	34.3	0.3	1
1	A	81	GLN	N	120.21	0.3	1
1	A	81	GLN	NE2	110.33	0.3	1
1	A	84	SER	H	7.72	0.03	1
1	A	84	SER	HA	4.24	0.03	1
1	A	84	SER	HB2	3.92	0.03	2
1	A	84	SER	HB3	3.96	0.03	2
1	A	84	SER	C	177.7	0.3	1
1	A	84	SER	CA	60.6	0.3	1
1	A	84	SER	CB	64.3	0.3	1
1	A	84	SER	N	113.1	0.3	1
1	A	85	ASN	H	7.66	0.03	1
1	A	85	ASN	HA	4.85	0.03	1
1	A	85	ASN	HB2	2.83	0.03	2
1	A	85	ASN	HB3	2.62	0.03	2
1	A	85	ASN	HD21	7.48	0.03	2
1	A	85	ASN	HD22	6.89	0.03	2
1	A	85	ASN	C	174.6	0.3	1
1	A	85	ASN	CA	53.6	0.3	1
1	A	85	ASN	CB	38.4	0.3	1
1	A	85	ASN	N	119.38	0.3	1
1	A	85	ASN	ND2	112.7	0.3	1
1	A	86	TYR	H	8.09	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	TYR	HA	4.37	0.03	1
1	A	86	TYR	HB2	3.01	0.03	2
1	A	86	TYR	HB3	2.95	0.03	2
1	A	86	TYR	HD1	7.08	0.03	3
1	A	86	TYR	HD2	7.08	0.03	3
1	A	86	TYR	HE1	6.75	0.03	3
1	A	86	TYR	HE2	6.75	0.03	3
1	A	86	TYR	CB	39.1	0.3	1
1	A	86	TYR	CD1	133.18	0.3	3
1	A	86	TYR	CD2	135.38	0.3	3
1	A	86	TYR	CE1	118.18	0.3	3
1	A	86	TYR	CE2	118.18	0.3	3
1	A	86	TYR	N	121.8	0.3	1
1	A	89	TYR	H	7.74	0.03	1
1	A	89	TYR	HA	4.54	0.03	1
1	A	89	TYR	HB2	3.06	0.03	2
1	A	89	TYR	HB3	2.82	0.03	2
1	A	89	TYR	HD1	7.14	0.03	3
1	A	89	TYR	HD2	7.14	0.03	3
1	A	89	TYR	HE1	6.78	0.03	3
1	A	89	TYR	HE2	6.78	0.03	3
1	A	89	TYR	CA	59.6	0.3	1
1	A	89	TYR	CB	39.5	0.3	1
1	A	89	TYR	CD1	133.38	0.3	3
1	A	89	TYR	CD2	133.38	0.3	3
1	A	89	TYR	CE1	118.18	0.3	3
1	A	89	TYR	CE2	118.18	0.3	3
1	A	89	TYR	N	117.7	0.3	1
1	A	92	PHE	H	8.0	0.03	1
1	A	92	PHE	HA	4.6	0.03	1
1	A	92	PHE	HB2	3.35	0.03	2
1	A	92	PHE	HB3	3.07	0.03	2
1	A	92	PHE	HD1	7.33	0.03	3
1	A	92	PHE	HD2	7.33	0.03	3
1	A	92	PHE	HE1	7.24	0.03	3
1	A	92	PHE	HE2	7.24	0.03	3
1	A	92	PHE	HZ	7.04	0.03	1
1	A	92	PHE	C	174.84	0.3	1
1	A	92	PHE	CA	58.9	0.3	1
1	A	92	PHE	CB	38.7	0.3	1
1	A	92	PHE	CD1	132.38	0.3	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	PHE	CD2	132.38	0.3	3
1	A	92	PHE	CE1	130.98	0.3	3
1	A	92	PHE	CE2	130.98	0.3	3
1	A	92	PHE	CZ	128.88	0.3	1
1	A	92	PHE	N	119.4	0.3	1
1	A	93	SER	H	8.21	0.03	1
1	A	93	SER	HA	4.42	0.03	1
1	A	93	SER	HB2	3.83	0.03	2
1	A	93	SER	HB3	3.83	0.03	2
1	A	93	SER	C	175.9	0.3	1
1	A	93	SER	CA	58.7	0.3	1
1	A	93	SER	CB	64.3	0.3	1
1	A	93	SER	N	114.8	0.3	1
1	A	94	ASN	H	8.42	0.03	1
1	A	94	ASN	HA	4.78	0.03	1
1	A	94	ASN	HB2	2.77	0.03	2
1	A	94	ASN	HB3	2.77	0.03	2
1	A	94	ASN	HD21	7.67	0.03	2
1	A	94	ASN	HD22	7.0	0.03	2
1	A	94	ASN	C	174.53	0.3	1
1	A	94	ASN	CA	53.7	0.3	1
1	A	94	ASN	CB	39.6	0.3	1
1	A	94	ASN	N	120.7	0.3	1
1	A	94	ASN	ND2	112.52	0.3	1
1	A	95	THR	H	8.04	0.03	1
1	A	95	THR	HA	4.29	0.03	1
1	A	95	THR	HB	4.17	0.03	1
1	A	95	THR	HG21	1.14	0.03	1
1	A	95	THR	HG22	1.14	0.03	1
1	A	95	THR	HG23	1.14	0.03	1
1	A	95	THR	C	175.21	0.3	1
1	A	95	THR	CA	62.3	0.3	1
1	A	95	THR	CB	70.2	0.3	1
1	A	95	THR	CG2	22.2	0.3	1
1	A	95	THR	N	114.11	0.3	1
1	A	96	TYR	H	8.19	0.03	1
1	A	96	TYR	HA	4.67	0.03	1
1	A	96	TYR	HB2	3.1	0.03	2
1	A	96	TYR	HB3	2.94	0.03	2
1	A	96	TYR	HD1	7.11	0.03	3
1	A	96	TYR	HD2	7.11	0.03	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	TYR	HE1	6.79	0.03	3
1	A	96	TYR	HE2	6.79	0.03	3
1	A	96	TYR	C	174.29	0.3	1
1	A	96	TYR	CA	58.4	0.3	1
1	A	96	TYR	CB	39.3	0.3	1
1	A	96	TYR	CD1	133.38	0.3	3
1	A	96	TYR	CD2	133.38	0.3	3
1	A	96	TYR	CE1	118.38	0.3	3
1	A	96	TYR	CE2	118.38	0.3	3
1	A	96	TYR	N	122.33	0.3	1
1	A	97	THR	H	8.12	0.03	1
1	A	97	THR	HA	4.37	0.03	1
1	A	97	THR	HB	4.28	0.03	1
1	A	97	THR	HG21	1.18	0.03	1
1	A	97	THR	HG22	1.18	0.03	1
1	A	97	THR	HG23	1.18	0.03	1
1	A	97	THR	C	176.0	0.3	1
1	A	97	THR	CA	62.0	0.3	1
1	A	97	THR	CB	70.6	0.3	1
1	A	97	THR	CG2	21.9	0.3	1
1	A	97	THR	N	115.1	0.3	1
1	A	98	ASP	H	8.33	0.03	1
1	A	98	ASP	HA	4.38	0.03	1
1	A	98	ASP	HB2	2.65	0.03	2
1	A	98	ASP	HB3	2.76	0.03	2
1	A	98	ASP	C	174.21	0.3	1
1	A	98	ASP	CA	55.5	0.3	1
1	A	98	ASP	CB	41.6	0.3	1
1	A	98	ASP	N	122.26	0.3	1
1	A	99	GLU	H	8.34	0.03	1
1	A	99	GLU	HA	4.22	0.03	1
1	A	99	GLU	HB2	2.06	0.03	2
1	A	99	GLU	HB3	1.96	0.03	2
1	A	99	GLU	HG2	2.27	0.03	2
1	A	99	GLU	HG3	2.27	0.03	2
1	A	99	GLU	C	176.7	0.3	1
1	A	99	GLU	CA	57.9	0.3	1
1	A	99	GLU	CB	30.6	0.3	1
1	A	99	GLU	CG	36.3	0.3	1
1	A	99	GLU	N	120.7	0.3	1
1	A	100	GLU	H	8.3	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	GLU	HA	4.22	0.03	1
1	A	100	GLU	HB2	2.04	0.03	2
1	A	100	GLU	HB3	2.04	0.03	2
1	A	100	GLU	HG2	2.27	0.03	2
1	A	100	GLU	HG3	2.27	0.03	2
1	A	100	GLU	C	177.22	0.3	1
1	A	100	GLU	CA	57.9	0.3	1
1	A	100	GLU	CB	30.5	0.3	1
1	A	100	GLU	CG	36.4	0.3	1
1	A	100	GLU	N	120.67	0.3	1
1	A	101	ASN	H	8.28	0.03	1
1	A	101	ASN	HA	4.67	0.03	1
1	A	101	ASN	HB2	2.82	0.03	2
1	A	101	ASN	HB3	2.8	0.03	2
1	A	101	ASN	HD21	7.68	0.03	2
1	A	101	ASN	HD22	6.88	0.03	2
1	A	101	ASN	C	176.89	0.3	1
1	A	101	ASN	CA	54.5	0.3	1
1	A	101	ASN	CB	39.5	0.3	1
1	A	101	ASN	N	118.35	0.3	1
1	A	101	ASN	ND2	113.3	0.3	1
1	A	102	GLU	H	8.3	0.03	1
1	A	102	GLU	HA	4.23	0.03	1
1	A	102	GLU	HB2	1.96	0.03	2
1	A	102	GLU	HB3	2.07	0.03	2
1	A	102	GLU	HG2	2.28	0.03	2
1	A	102	GLU	HG3	2.28	0.03	2
1	A	102	GLU	C	175.7	0.3	1
1	A	102	GLU	CA	58.0	0.3	1
1	A	102	GLU	CB	30.5	0.3	1
1	A	102	GLU	CG	36.6	0.3	1
1	A	102	GLU	N	120.48	0.3	1
1	A	103	THR	H	8.05	0.03	1
1	A	103	THR	HA	4.2	0.03	1
1	A	103	THR	HB	4.22	0.03	1
1	A	103	THR	HG21	1.21	0.03	1
1	A	103	THR	HG22	1.21	0.03	1
1	A	103	THR	HG23	1.21	0.03	1
1	A	103	THR	C	177.12	0.3	1
1	A	103	THR	CA	63.8	0.3	1
1	A	103	THR	CB	69.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	THR	CG2	22.2	0.3	1
1	A	103	THR	N	114.11	0.3	1
1	A	104	LEU	H	8.0	0.03	1
1	A	104	LEU	HA	4.27	0.03	1
1	A	104	LEU	HB2	1.68	0.03	2
1	A	104	LEU	HB3	1.6	0.03	2
1	A	104	LEU	HD11	0.89	0.03	2
1	A	104	LEU	HD12	0.89	0.03	2
1	A	104	LEU	HD13	0.89	0.03	2
1	A	104	LEU	HD21	0.85	0.03	2
1	A	104	LEU	HD22	0.85	0.03	2
1	A	104	LEU	HD23	0.85	0.03	2
1	A	104	LEU	HG	1.62	0.03	1
1	A	104	LEU	C	175.02	0.3	1
1	A	104	LEU	CA	56.6	0.3	1
1	A	104	LEU	CB	42.5	0.3	1
1	A	104	LEU	CD1	25.5	0.3	1
1	A	104	LEU	CD2	24.1	0.3	1
1	A	104	LEU	CG	27.5	0.3	1
1	A	104	LEU	N	122.36	0.3	1
1	A	105	ILE	H	7.87	0.03	1
1	A	105	ILE	HA	4.07	0.03	1
1	A	105	ILE	HB	1.84	0.03	1
1	A	105	ILE	HD11	0.81	0.03	1
1	A	105	ILE	HD12	0.81	0.03	1
1	A	105	ILE	HD13	0.81	0.03	1
1	A	105	ILE	HG12	1.12	0.03	1
1	A	105	ILE	HG13	1.47	0.03	1
1	A	105	ILE	HG21	0.86	0.03	1
1	A	105	ILE	HG22	0.86	0.03	1
1	A	105	ILE	HG23	0.86	0.03	1
1	A	105	ILE	C	177.43	0.3	1
1	A	105	ILE	CA	61.9	0.3	1
1	A	105	ILE	CB	38.9	0.3	1
1	A	105	ILE	CD1	13.8	0.3	1
1	A	105	ILE	CG1	28.1	0.3	1
1	A	105	ILE	CG2	17.7	0.3	1
1	A	105	ILE	N	118.8	0.3	1
1	A	106	ASN	H	8.07	0.03	1
1	A	106	ASN	C	178.44	0.3	1
1	A	106	ASN	N	120.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	LEU	H	8.53	0.03	1
1	A	107	LEU	HA	4.07	0.03	1
1	A	107	LEU	HB2	1.57	0.03	2
1	A	107	LEU	HB3	1.7	0.03	2
1	A	107	LEU	HD11	0.88	0.03	2
1	A	107	LEU	HD12	0.88	0.03	2
1	A	107	LEU	HD13	0.88	0.03	2
1	A	107	LEU	HD21	0.79	0.03	2
1	A	107	LEU	HD22	0.79	0.03	2
1	A	107	LEU	HD23	0.79	0.03	2
1	A	107	LEU	C	176.39	0.3	1
1	A	107	LEU	CA	57.3	0.3	1
1	A	107	LEU	CB	42.2	0.3	1
1	A	107	LEU	CD1	25.7	0.3	1
1	A	107	LEU	CD2	24.2	0.3	1
1	A	107	LEU	N	125.54	0.3	1
1	A	108	GLU	H	8.38	0.03	1
1	A	108	GLU	HA	4.06	0.03	1
1	A	108	GLU	HB2	2.12	0.03	2
1	A	108	GLU	HB3	2.07	0.03	2
1	A	108	GLU	HG2	2.36	0.03	2
1	A	108	GLU	HG3	2.28	0.03	2
1	A	108	GLU	C	177.88	0.3	1
1	A	108	GLU	CA	60.5	0.3	1
1	A	108	GLU	CB	29.3	0.3	1
1	A	108	GLU	CG	37.1	0.3	1
1	A	108	GLU	N	120.2	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	186	-1.23 ± 0.13	Should be checked
$^{13}C_{\beta}$	182	-0.16 ± 0.04	None needed (< 0.5 ppm)
$^{13}C'$	170	-0.69 ± 0.19	Should be applied
^{15}N	188	-0.08 ± 0.11	None needed (< 0.5 ppm)

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 93%, i.e. 1810 atoms were assigned a chemical shift out of a possible 1937. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	668/680 (98%)	274/274 (100%)	260/272 (96%)	134/134 (100%)
Sidechain	1074/1169 (92%)	732/760 (96%)	330/373 (88%)	12/36 (33%)
Aromatic	68/88 (77%)	34/42 (81%)	34/38 (89%)	0/8 (0%)
Overall	1810/1937 (93%)	1040/1076 (97%)	624/683 (91%)	146/178 (82%)

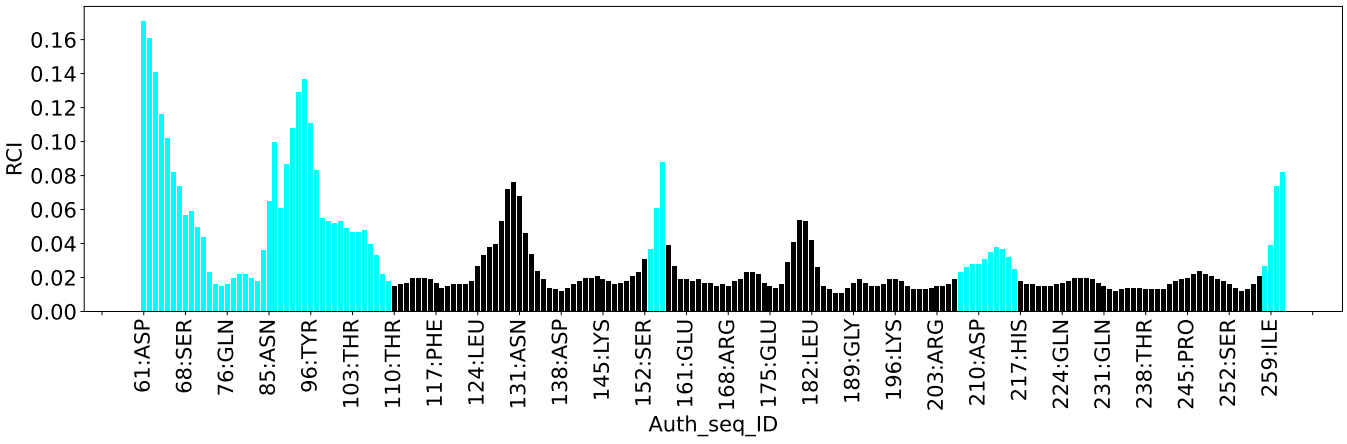
7.1.4 Statistically unusual chemical shifts

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:



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	3108
Intra-residue (|i-j|=0)	846
Sequential (|i-j|=1)	732
Medium range (|i-j|>1 and |i-j|<5)	781
Long range (|i-j|≥5)	555
Inter-chain	0
Hydrogen bond restraints	194
Disulfide bond restraints	0
Total dihedral-angle restraints	254
Number of unmapped restraints	7
Number of restraints per residue	16.5
Number of long range restraints per residue[1]	2.7

[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)	2.4	0.2
0.2-0.5 (Medium)	1.1	0.23
>0.5 (Large)	None	None

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)

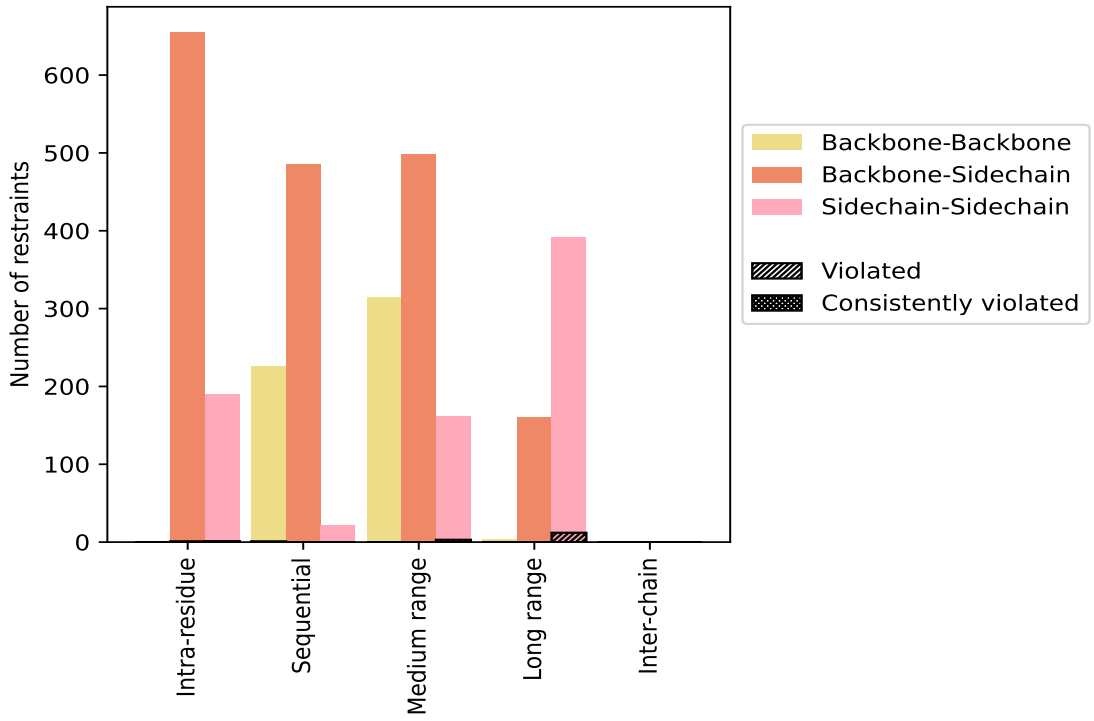
9.1 Summary of distance violations (i)

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)	846	27.2	2	0.2	0.1	1	0.1	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	655	21.1	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	190	6.1	1	0.5	0.0	1	0.5	0.0
Sequential (|i-j|=1)	732	23.6	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	226	7.3	1	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	485	15.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	0.7	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	781	25.1	3	0.4	0.1	0	0.0	0.0
Backbone-Backbone	315	10.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	304	9.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	162	5.2	3	1.9	0.1	0	0.0	0.0
Long range (|i-j|≥5)	555	17.9	12	2.2	0.4	0	0.0	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	160	5.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	392	12.6	12	3.1	0.4	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	194	6.2	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	3108	100.0	18	0.6	0.6	1	0.0	0.0
Backbone-Backbone	545	17.5	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	1798	57.9	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	765	24.6	16	2.1	0.5	1	0.1	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



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	1	0	0	6	0	7	0.14	0.23	0.04	0.12
2	1	0	0	1	0	2	0.22	0.23	0.02	0.22
3	1	0	0	6	0	7	0.15	0.23	0.03	0.14
4	1	0	0	0	0	1	0.23	0.23	0.0	0.23
5	1	0	0	1	0	2	0.23	0.23	0.0	0.23
6	2	0	3	1	0	6	0.15	0.23	0.04	0.14
7	1	0	1	6	0	8	0.15	0.23	0.04	0.13
8	1	0	2	0	0	3	0.16	0.23	0.05	0.13
9	1	0	0	1	0	2	0.22	0.23	0.01	0.22
10	1	0	0	1	0	2	0.2	0.23	0.03	0.2

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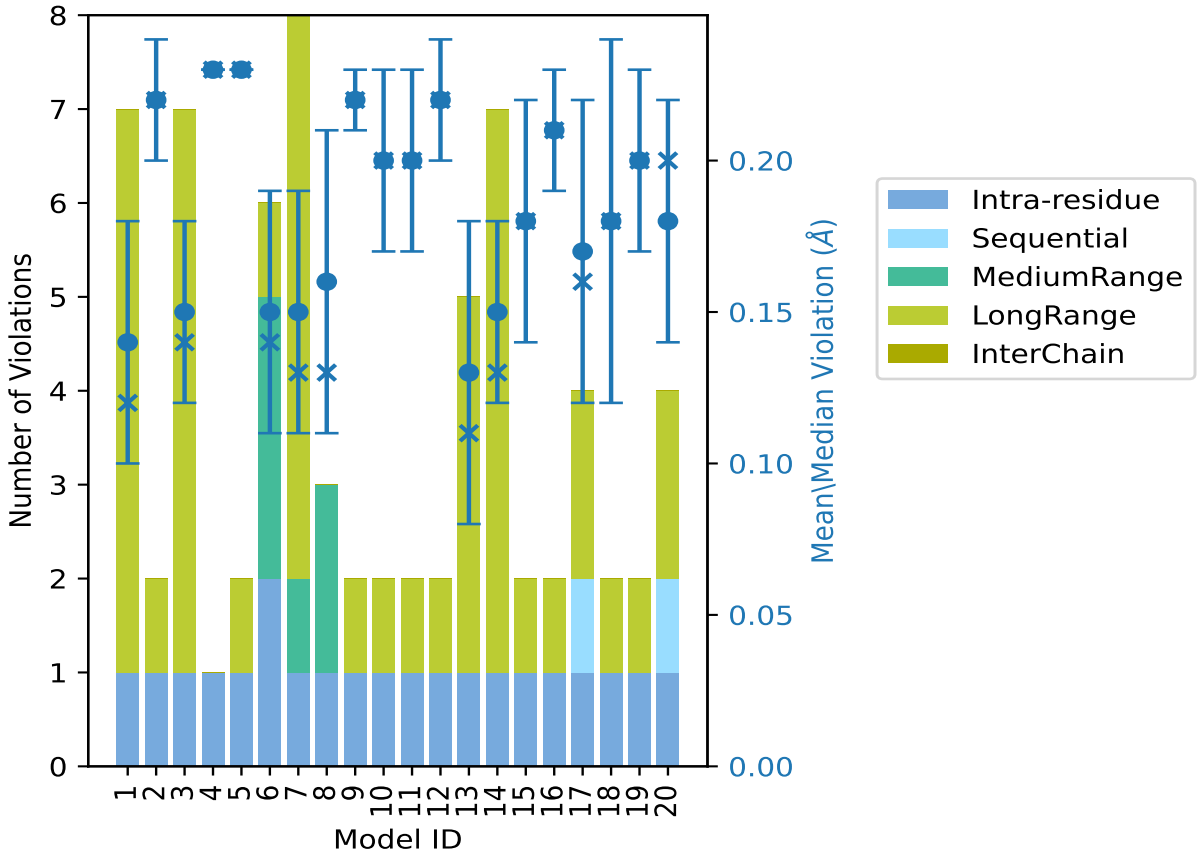
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	1	0	0	1	0	2	0.2	0.23	0.03	0.2
12	1	0	0	1	0	2	0.22	0.23	0.02	0.22
13	1	0	0	4	0	5	0.13	0.23	0.05	0.11
14	1	0	0	6	0	7	0.15	0.23	0.03	0.13
15	1	0	0	1	0	2	0.18	0.23	0.04	0.18
16	1	0	0	1	0	2	0.21	0.23	0.02	0.21
17	1	1	0	2	0	4	0.17	0.23	0.05	0.16
18	1	0	0	1	0	2	0.18	0.23	0.06	0.18
19	1	0	0	1	0	2	0.2	0.23	0.03	0.2
20	1	1	0	2	0	4	0.18	0.23	0.04	0.2

[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

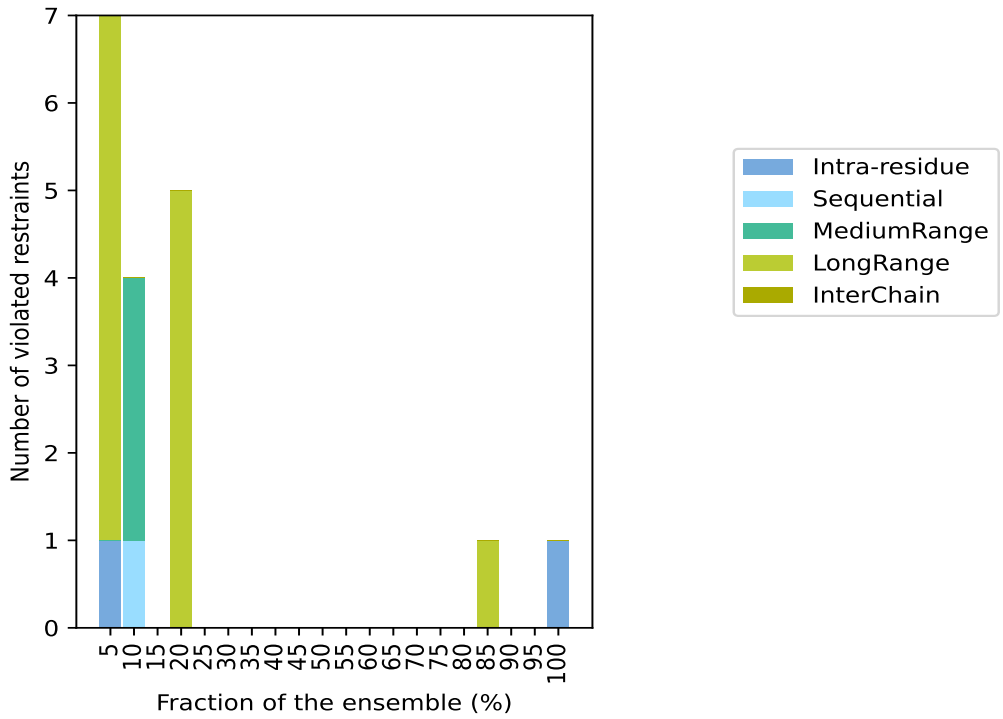
9.3 Distance violation statistics for the ensemble (i)

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, 2896(IR:844, SQ:731, MR:778, LR:543, 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]	%
1	0	0	6	0	7	1	5.0
0	1	3	0	0	4	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	5	0	5	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	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	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	0	0	1	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

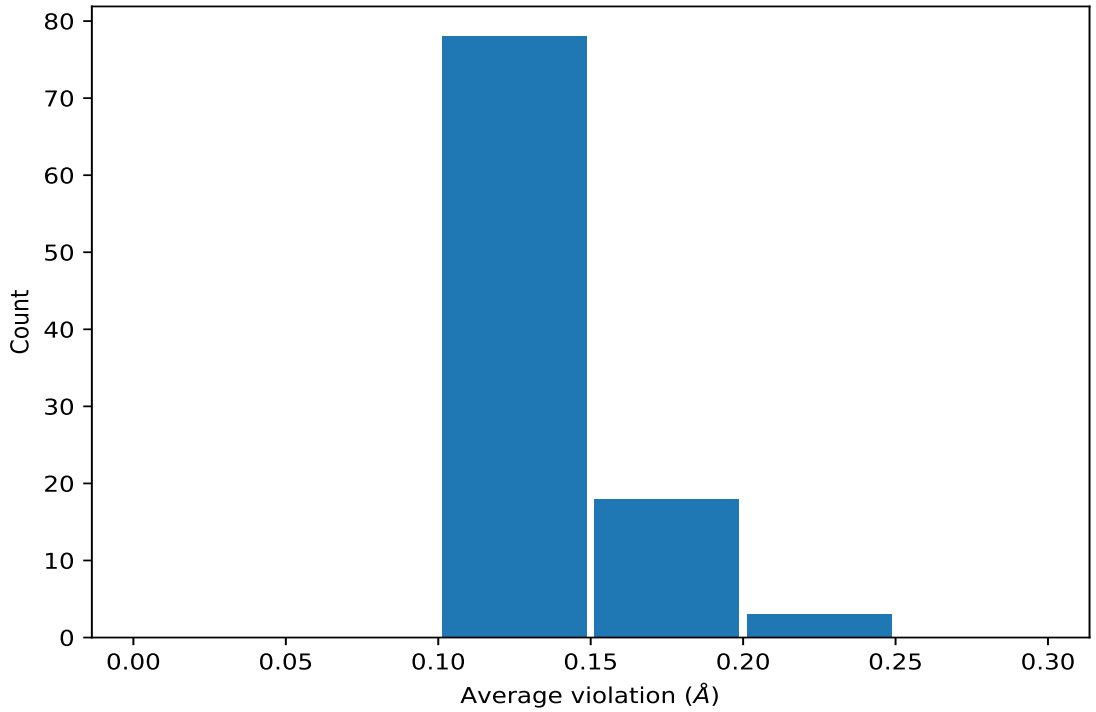
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

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)
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	20	0.23	0.0	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	20	0.23	0.0	0.23
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD11	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD12	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD13	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD21	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD22	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG11	1:190:A:LEU:HD23	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD11	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD12	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD13	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD21	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD22	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG12	1:190:A:LEU:HD23	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD11	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD12	17	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD13	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD21	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD22	17	0.17	0.03	0.17
(1,636)	1:139:A:VAL:HG13	1:190:A:LEU:HD23	17	0.17	0.03	0.17
(1,2473)	1:234:A:LEU:HD21	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD21	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD21	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD22	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD22	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD22	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD23	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD23	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2473)	1:234:A:LEU:HD23	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD21	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD21	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD21	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD22	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD22	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD22	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD23	1:255:A:LEU:HD21	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD23	1:255:A:LEU:HD22	4	0.13	0.01	0.13
(1,2474)	1:234:A:LEU:HD23	1:255:A:LEU:HD23	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD21	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD21	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD21	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD22	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD22	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD22	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD23	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD23	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2825)	1:255:A:LEU:HD23	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD21	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD21	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD21	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD22	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD22	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD22	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD23	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD23	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2826)	1:255:A:LEU:HD23	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD21	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD21	1:234:A:LEU:HD22	4	0.13	0.01	0.13

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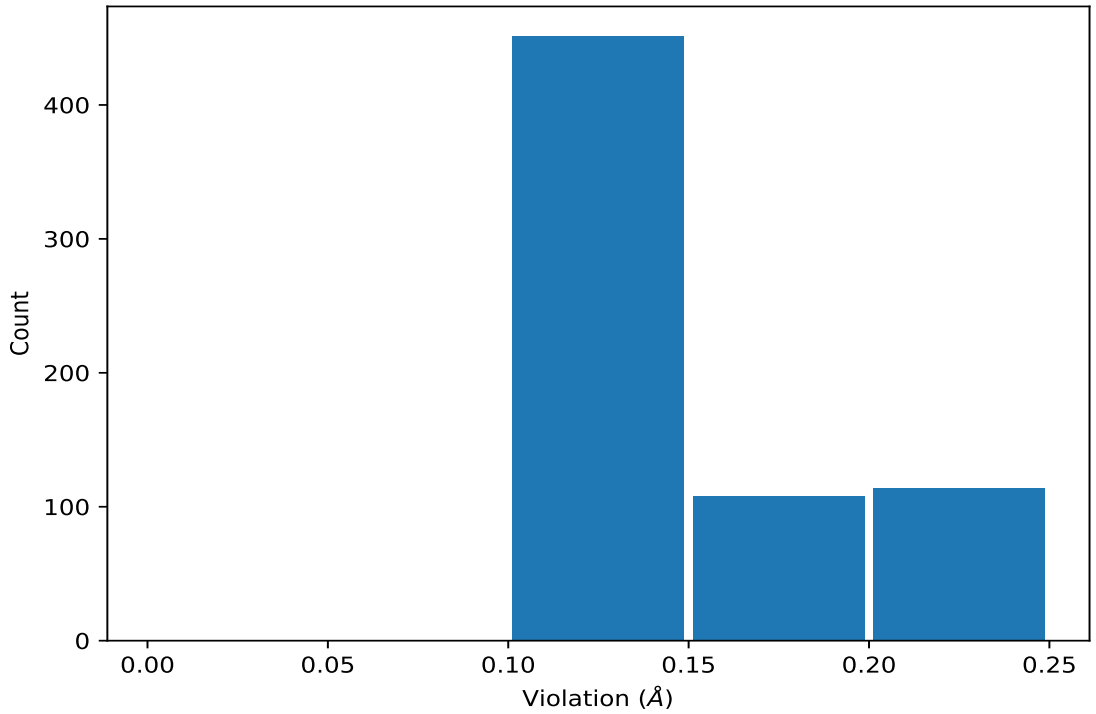
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2827)	1:255:A:LEU:HD21	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD22	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD22	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD22	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD23	1:234:A:LEU:HD21	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD23	1:234:A:LEU:HD22	4	0.13	0.01	0.13
(1,2827)	1:255:A:LEU:HD23	1:234:A:LEU:HD23	4	0.13	0.01	0.13
(1,4)	1:109:A:LYS:H	1:110:A:THR:H	2	0.2	0.0	0.2
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD11	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD12	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD13	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD21	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD22	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE2	1:140:A:LEU:HD23	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD11	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD12	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD13	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD21	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD22	2	0.14	0.01	0.14
(1,582)	1:137:A:LYS:HE3	1:140:A:LEU:HD23	2	0.14	0.01	0.14
(1,668)	1:140:A:LEU:HD11	1:137:A:LYS:HE2	2	0.14	0.01	0.14

[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)
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	1	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	1	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	2	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	2	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	3	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	3	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	4	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	4	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	5	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	5	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	6	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	6	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	7	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	7	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	8	0.23
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	8	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:167:A:LYS:HG3	1:167:A:LYS:HG2	9	0.23
(1,1184)	1:167:A:LYS:HG2	1:167:A:LYS:HG3	10	0.23

10 Dihedral-angle violation analysis

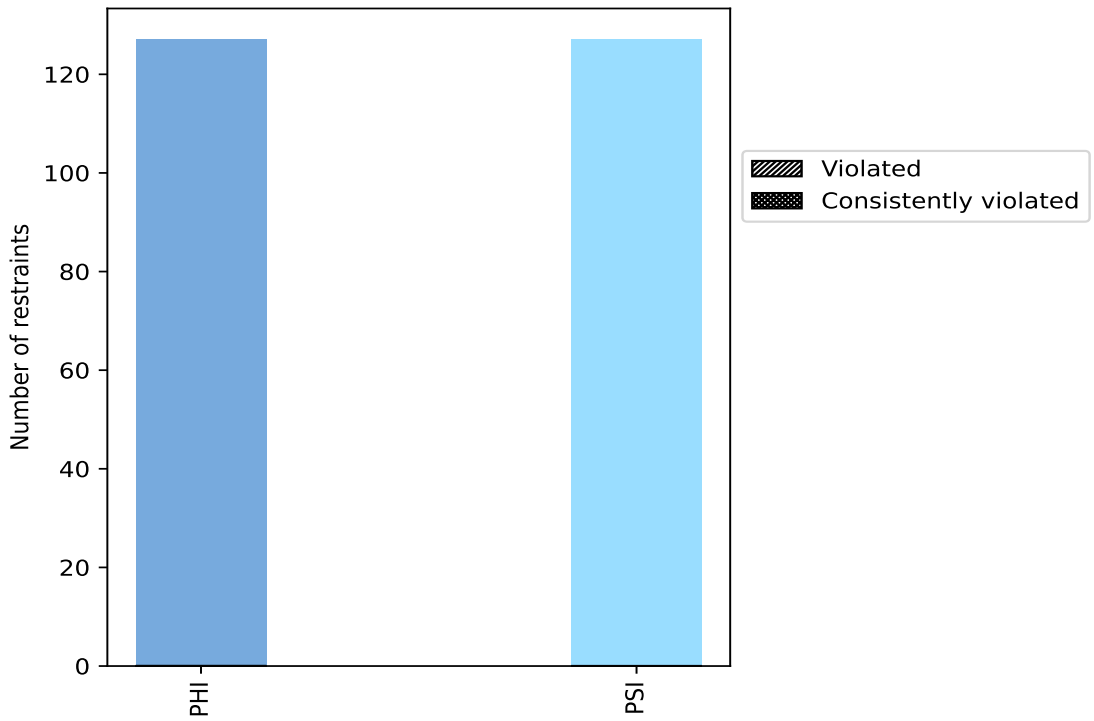
10.1 Summary of dihedral-angle violations

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	127	50.0	0	0.0	0.0	0	0.0	0.0
PSI	127	50.0	0	0.0	0.0	0	0.0	0.0
Total	254	100.0	0	0.0	0.0	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)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble (i)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble (i)

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found