



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 8DDC
BMRB ID : 31026
Title : Intramembrane recognition between transmembrane domains of IL-7R and common gamma chain
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Deposited on : 2022-06-17

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

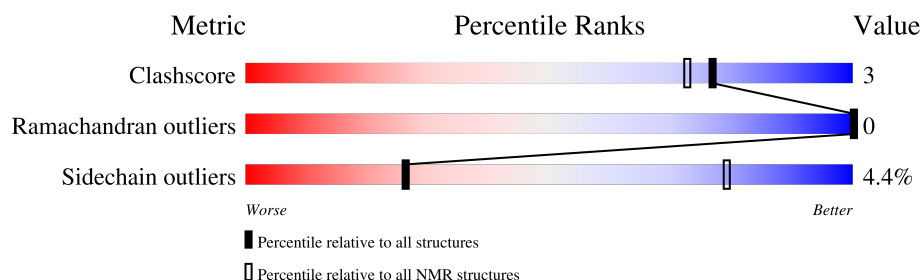
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	34	
2	B	31	

2 Ensemble composition and analysis

This entry contains 15 models. Model 14 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:268-A:279 (12)	0.11	8
2	B:250-B:264 (15)	0.15	14

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1076 atoms, of which 555 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					Trace
1	A	34	Total	C	H	N	O	0
			561	188	286	39	48	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	VAL	MET	engineered mutation	UNP P34902
A	282	PHE	CYS	engineered mutation	UNP P34902

- Molecule 2 is a protein called Interleukin-7 receptor subunit alpha.

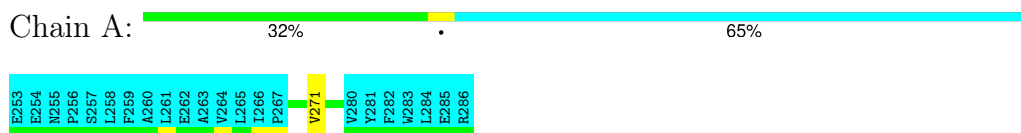
Mol	Chain	Residues	Atoms					Trace
2	B	31	Total	C	H	N	O	0
			515	171	269	37	38	

4 Residue-property plots [i](#)

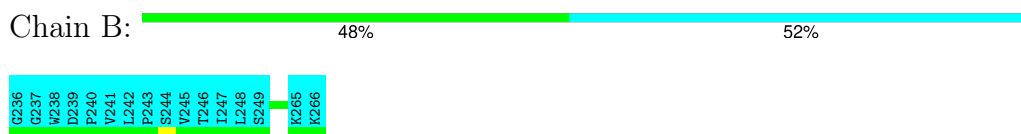
4.1 Average score per residue in the NMR ensemble

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: Cytokine receptor common subunit gamma



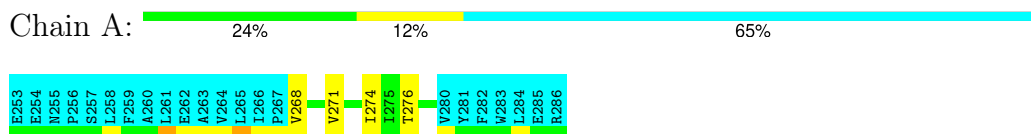
- Molecule 2: Interleukin-7 receptor subunit alpha



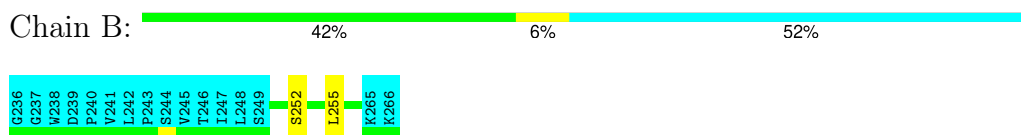
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: Cytokine receptor common subunit gamma



- Molecule 2: Interleukin-7 receptor subunit alpha



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	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	654
Number of shifts mapped to atoms	654
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	87	102	102	1±1
2	B	126	139	138	1±1
All	All	3195	3615	3600	19

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 3.

5 of 13 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:250:LEU:O	2:B:250:LEU:HD13	0.52	2.05	10	2
1:A:274:ILE:HD11	2:B:255:LEU:O	0.51	2.05	4	4
2:B:251:PHE:CE1	2:B:255:LEU:HD11	0.50	2.41	15	2
2:B:250:LEU:O	2:B:250:LEU:HD23	0.44	2.13	2	1
2:B:255:LEU:HD23	2:B:258:ILE:HD12	0.44	1.89	15	2

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	12/34 (35%)	12±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	15/31 (48%)	15±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	405/975 (42%)	405 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	10/30 (33%)	10±1 (96±7%)	0±1 (4±7%)	29	82
2	B	14/28 (50%)	13±1 (95±5%)	1±1 (5±5%)	24	77
All	All	360/870 (41%)	344 (96%)	16 (4%)	26	79

5 of 8 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)
2	B	252	SER	4
1	A	276	THR	2
2	B	250	LEU	2
2	B	254	PHE	2
1	A	279	PHE	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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 72% for the well-defined parts and 58% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS.tab*

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	654
Number of shifts mapped to atoms	654
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	258	LEU	HD12	0.91	0.010	.
1	A	258	LEU	HD13	0.91	0.010	.
1	A	258	LEU	HD22	0.84	0.010	.
1	A	258	LEU	HD23	0.84	0.010	.
1	A	263	ALA	HB2	1.35	0.010	1
1	A	263	ALA	HB3	1.35	0.010	1
1	A	264	VAL	HG12	0.99	0.010	.
1	A	264	VAL	HG13	0.99	0.010	.
1	A	264	VAL	HG22	0.89	0.002	.
1	A	264	VAL	HG23	0.89	0.002	.
1	A	266	ILE	HG22	0.80	0.002	1
1	A	266	ILE	HG23	0.80	0.002	1
1	A	266	ILE	HD12	0.86	0.020	1
1	A	266	ILE	HD13	0.86	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	268	VAL	HG12	1.02	0.005	.
1	A	268	VAL	HG13	1.02	0.005	.
1	A	270	THR	HG22	1.08	0.002	1
1	A	270	THR	HG23	1.08	0.002	1
1	A	271	VAL	HG12	1.01	0.002	.
1	A	271	VAL	HG13	1.01	0.002	.
1	A	271	VAL	HG22	0.87	0.002	.
1	A	271	VAL	HG23	0.87	0.002	.
1	A	273	LEU	HD12	0.84	0.002	.
1	A	273	LEU	HD13	0.84	0.002	.
1	A	273	LEU	HD22	0.84	0.002	.
1	A	273	LEU	HD23	0.84	0.002	.
1	A	274	ILE	HG22	0.85	0.002	1
1	A	274	ILE	HG23	0.85	0.002	1
1	A	274	ILE	HD12	0.76	0.002	1
1	A	274	ILE	HD13	0.76	0.002	1
1	A	275	ILE	HG22	0.85	0.002	1
1	A	275	ILE	HG23	0.85	0.002	1
1	A	275	ILE	HD12	0.75	0.002	1
1	A	275	ILE	HD13	0.75	0.002	1
1	A	277	LEU	HD12	0.81	0.002	.
1	A	277	LEU	HD13	0.81	0.002	.
1	A	277	LEU	HD22	0.81	0.002	.
1	A	277	LEU	HD23	0.81	0.002	.
1	A	278	ILE	HG22	0.94	0.002	1
1	A	278	ILE	HG23	0.94	0.002	1
1	A	278	ILE	HD12	0.78	0.002	1
1	A	278	ILE	HD13	0.78	0.002	1
1	A	280	VAL	HG12	1.16	0.002	.
1	A	280	VAL	HG13	1.16	0.002	.
1	A	280	VAL	HG22	1.01	0.002	.
1	A	280	VAL	HG23	1.01	0.002	.
1	A	284	LEU	HD12	0.87	0.002	.
1	A	284	LEU	HD13	0.87	0.002	.
1	A	284	LEU	HD22	0.81	0.002	.
1	A	284	LEU	HD23	0.81	0.002	.
1	B	242	LEU	HD12	0.92	0.010	.
1	B	242	LEU	HD13	0.92	0.010	.
1	B	242	LEU	HD22	0.87	0.010	.
1	B	242	LEU	HD23	0.87	0.010	.
1	B	245	VAL	HG12	0.91	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	245	VAL	HG13	0.91	0.010	.
1	B	245	VAL	HG22	1.04	0.010	.
1	B	245	VAL	HG23	1.04	0.010	.
1	B	246	THR	HG22	1.11	0.010	1
1	B	246	THR	HG23	1.11	0.010	1
1	B	247	ILE	HG22	0.82	0.010	1
1	B	247	ILE	HG23	0.82	0.010	1
1	B	247	ILE	HD12	0.80	0.010	1
1	B	247	ILE	HD13	0.80	0.010	1
1	B	248	LEU	HD12	0.88	0.020	.
1	B	248	LEU	HD13	0.88	0.020	.
1	B	248	LEU	HD22	0.83	0.010	.
1	B	248	LEU	HD23	0.83	0.010	.
1	B	250	LEU	HD12	0.78	0.010	.
1	B	250	LEU	HD13	0.78	0.010	.
1	B	250	LEU	HD22	0.76	0.010	.
1	B	250	LEU	HD23	0.76	0.010	.
1	B	253	VAL	HG12	0.83	0.010	.
1	B	253	VAL	HG13	0.83	0.010	.
1	B	253	VAL	HG22	1.01	0.010	.
1	B	253	VAL	HG23	1.01	0.010	.
1	B	255	LEU	HD12	0.72	0.020	.
1	B	255	LEU	HD13	0.72	0.020	.
1	B	255	LEU	HD22	0.80	0.020	.
1	B	255	LEU	HD23	0.80	0.020	.
1	B	256	LEU	HD12	0.82	0.020	.
1	B	256	LEU	HD13	0.82	0.020	.
1	B	256	LEU	HD22	0.82	0.020	.
1	B	256	LEU	HD23	0.82	0.020	.
1	B	257	VAL	HG12	0.88	0.010	.
1	B	257	VAL	HG13	0.88	0.010	.
1	B	257	VAL	HG22	1.01	0.010	.
1	B	257	VAL	HG23	1.01	0.010	.
1	B	258	ILE	HG22	0.78	0.010	1
1	B	258	ILE	HG23	0.78	0.010	1
1	B	258	ILE	HD12	0.51	0.010	1
1	B	258	ILE	HD13	0.51	0.010	1
1	B	259	LEU	HD12	0.80	0.010	.
1	B	259	LEU	HD13	0.80	0.010	.
1	B	259	LEU	HD22	0.78	0.020	.
1	B	259	LEU	HD23	0.78	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	260	ALA	HB2	1.42	0.010	1
1	A	260	ALA	HB3	1.42	0.010	1
1	B	262	VAL	HG12	0.95	0.010	.
1	B	262	VAL	HG13	0.95	0.010	.
1	B	262	VAL	HG22	1.09	0.010	.
1	B	262	VAL	HG23	1.09	0.010	.
1	B	263	LEU	HD12	0.72	0.010	.
1	B	263	LEU	HD13	0.72	0.010	.
1	B	263	LEU	HD22	0.76	0.010	.
1	B	263	LEU	HD23	0.76	0.010	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	52	0.04 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	1	—	None (insufficient data)
$^{13}\text{C}'$	50	-1.82 ± 0.07	Should be applied
^{15}N	50	0.57 ± 0.20	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 72%, i.e. 298 atoms were assigned a chemical shift out of a possible 414. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	129/137 (94%)	52/56 (93%)	51/54 (94%)	26/27 (96%)
Sidechain	164/227 (72%)	132/157 (84%)	32/70 (46%)	0/0 (—%)
Aromatic	5/50 (10%)	5/25 (20%)	0/22 (0%)	0/3 (0%)
Overall	298/414 (72%)	189/238 (79%)	83/146 (57%)	26/30 (87%)

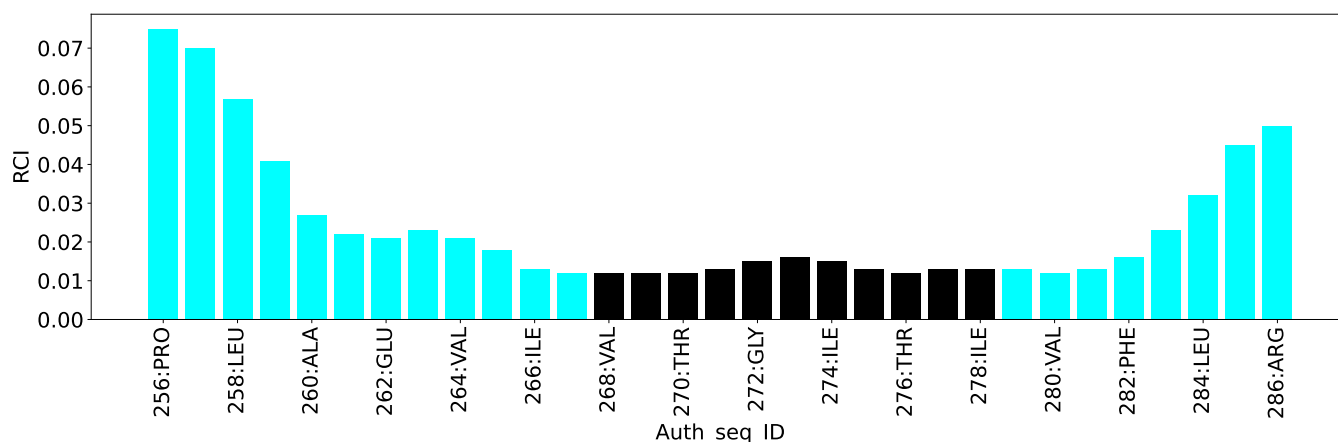
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

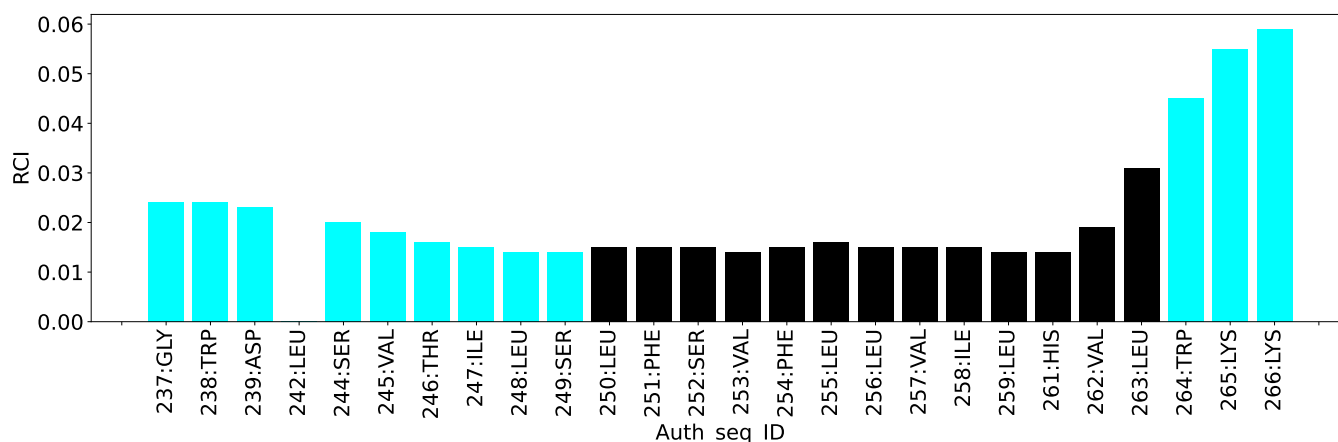
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	248
Intra-residue ($ i-j =0$)	47
Sequential ($ i-j =1$)	101
Medium range ($ i-j >1$ and $ i-j <5$)	76
Long range ($ i-j \geq 5$)	2
Inter-chain	22
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	94
Number of unmapped restraints	0
Number of restraints per residue	5.3
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	14.2	0.2
0.2-0.5 (Medium)	9.2	0.49
>0.5 (Large)	0.3	0.57

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)	2.7	1.75
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

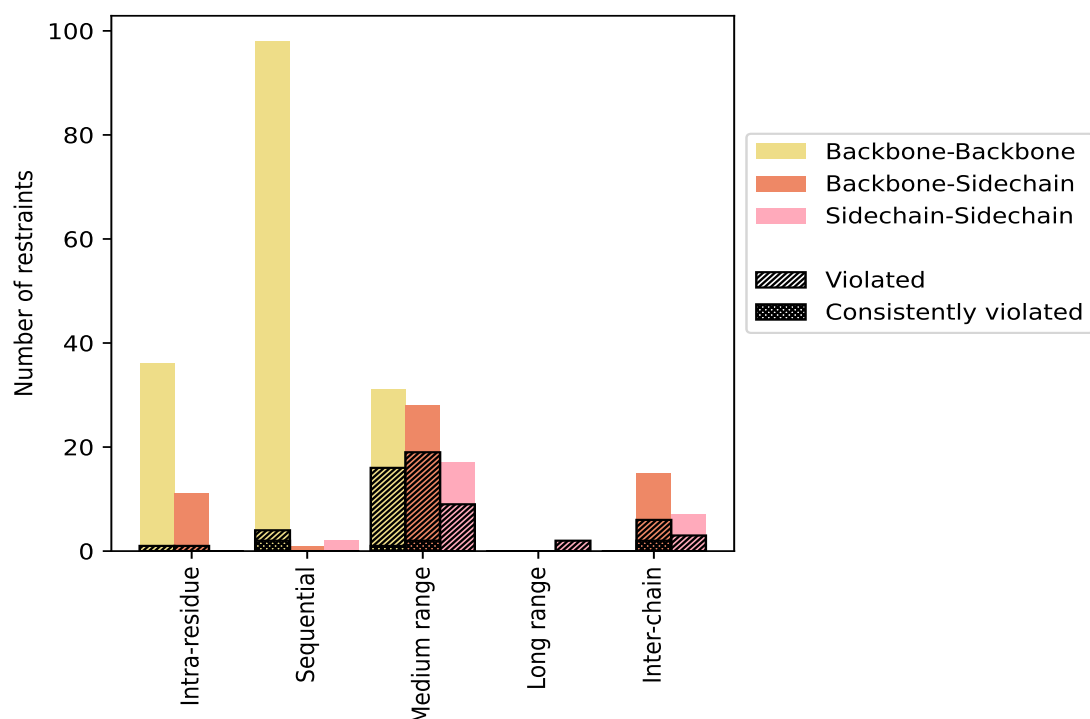
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	47	19.0	2	4.3	0.8	0	0.0	0.0
Backbone-Backbone	36	14.5	1	2.8	0.4	0	0.0	0.0
Backbone-Sidechain	11	4.4	1	9.1	0.4	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	101	40.7	4	4.0	1.6	2	2.0	0.8
Backbone-Backbone	98	39.5	4	4.1	1.6	2	2.0	0.8
Backbone-Sidechain	1	0.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	2	0.8	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	76	30.6	44	57.9	17.7	3	3.9	1.2
Backbone-Backbone	31	12.5	16	51.6	6.5	1	3.2	0.4
Backbone-Sidechain	28	11.3	19	67.9	7.7	2	7.1	0.8
Sidechain-Sidechain	17	6.9	9	52.9	3.6	0	0.0	0.0
Long range (i-j ≥5)	2	0.8	2	100.0	0.8	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	2	0.8	2	100.0	0.8	0	0.0	0.0
Inter-chain	22	8.9	9	40.9	3.6	2	9.1	0.8
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	15	6.0	6	40.0	2.4	2	13.3	0.8
Sidechain-Sidechain	7	2.8	3	42.9	1.2	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	248	100.0	61	24.6	24.6	7	2.8	2.8
Backbone-Backbone	165	66.5	21	12.7	8.5	3	1.8	1.2
Backbone-Sidechain	55	22.2	26	47.3	10.5	4	7.3	1.6
Sidechain-Sidechain	28	11.3	14	50.0	5.6	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	3	17	1	3	24	0.2	0.48	0.08	0.2
2	0	2	14	1	5	22	0.21	0.47	0.1	0.16
3	1	3	16	0	6	26	0.2	0.51	0.1	0.18
4	0	2	18	1	5	26	0.2	0.49	0.11	0.17
5	0	4	21	1	3	29	0.23	0.49	0.11	0.19
6	0	3	18	1	4	26	0.22	0.56	0.11	0.19
7	0	2	16	1	5	24	0.22	0.49	0.1	0.2
8	0	2	11	2	5	20	0.21	0.48	0.11	0.18
9	0	2	16	0	4	22	0.2	0.47	0.11	0.17
10	0	3	18	1	5	27	0.2	0.49	0.09	0.16

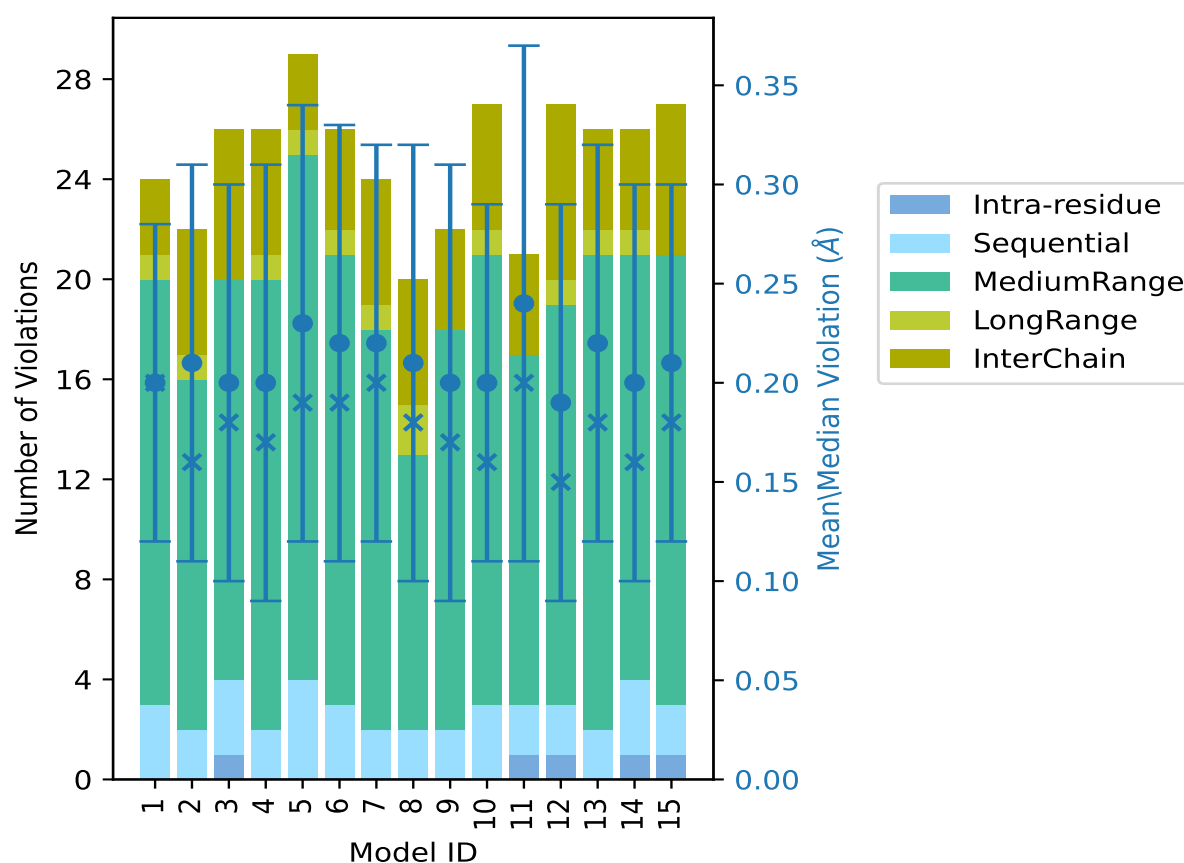
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	2	14	0	4	21	0.24	0.57	0.13	0.2
12	1	2	16	1	7	27	0.19	0.49	0.1	0.15
13	0	2	19	1	4	26	0.22	0.49	0.1	0.18
14	1	3	17	1	4	26	0.2	0.49	0.1	0.16
15	1	2	18	0	6	27	0.21	0.49	0.09	0.18

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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 ⓘ

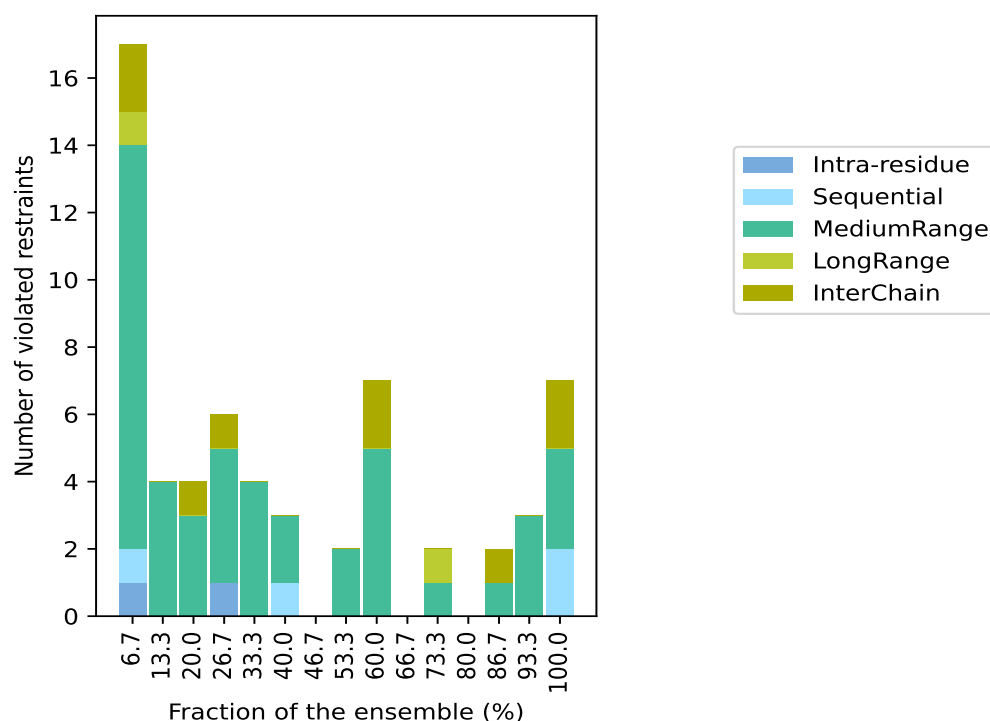
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 187(IR:45, SQ:97, MR:32, LR:0, IC:13) restraints are not 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	1	12	1	2	17	1	6.7
0	0	4	0	0	4	2	13.3
0	0	3	0	1	4	3	20.0
1	0	4	0	1	6	4	26.7
0	0	4	0	0	4	5	33.3
0	1	2	0	0	3	6	40.0
0	0	0	0	0	0	7	46.7
0	0	2	0	0	2	8	53.3
0	0	5	0	2	7	9	60.0
0	0	0	0	0	0	10	66.7
0	0	1	1	0	2	11	73.3
0	0	0	0	0	0	12	80.0
0	0	1	0	1	2	13	86.7
0	0	3	0	0	3	14	93.3
0	2	3	0	2	7	15	100.0

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

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

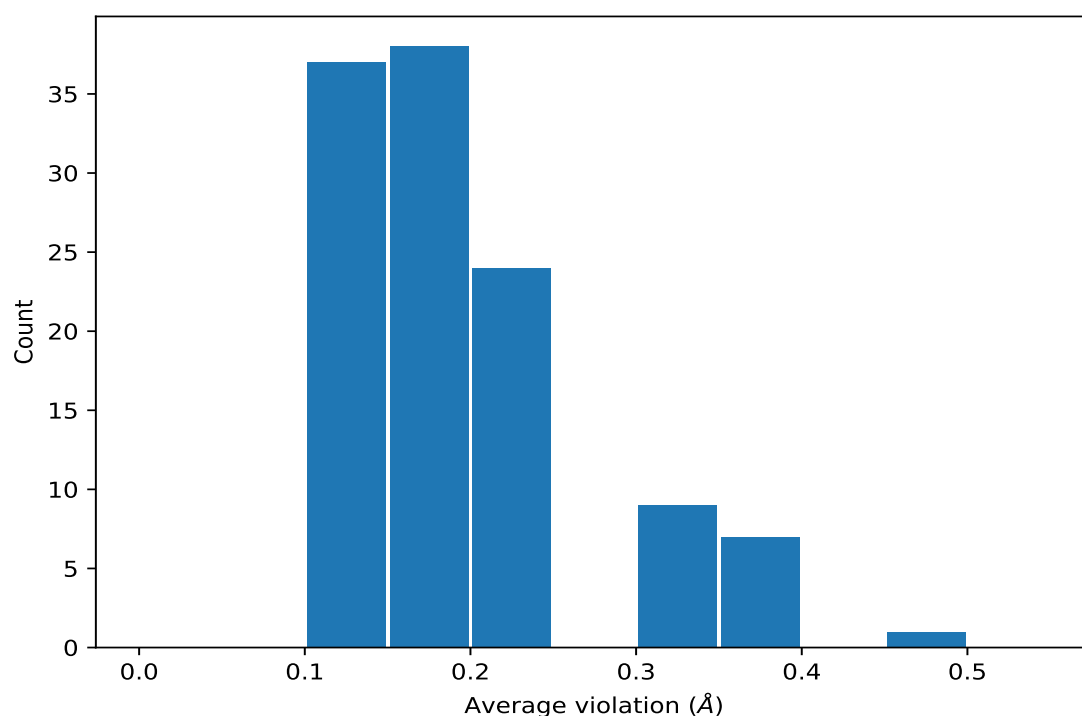
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the 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)
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	15	0.49	0.01	0.49
(1,247)	2:266:B:LYS:H	2:265:B:LYS:HA	15	0.39	0.06	0.35
(1,43)	1:264:A:VAL:HG11	1:262:A:GLU:HA	15	0.35	0.08	0.36
(1,43)	1:264:A:VAL:HG12	1:262:A:GLU:HA	15	0.35	0.08	0.36
(1,43)	1:264:A:VAL:HG13	1:262:A:GLU:HA	15	0.35	0.08	0.36
(1,26)	1:258:A:LEU:HD11	1:262:A:GLU:H	15	0.33	0.04	0.33
(1,26)	1:258:A:LEU:HD12	1:262:A:GLU:H	15	0.33	0.04	0.33
(1,26)	1:258:A:LEU:HD13	1:262:A:GLU:H	15	0.33	0.04	0.33
(1,12)	1:278:A:ILE:H	2:258:B:ILE:HG21	15	0.2	0.03	0.2
(1,12)	1:278:A:ILE:H	2:258:B:ILE:HG22	15	0.2	0.03	0.2
(1,12)	1:278:A:ILE:H	2:258:B:ILE:HG23	15	0.2	0.03	0.2
(1,19)	2:258:B:ILE:HG21	1:278:A:ILE:H	15	0.2	0.03	0.2
(1,19)	2:258:B:ILE:HG22	1:278:A:ILE:H	15	0.2	0.03	0.2
(1,19)	2:258:B:ILE:HG23	1:278:A:ILE:H	15	0.2	0.03	0.2
(1,223)	2:262:B:VAL:H	2:259:B:LEU:HA	15	0.19	0.06	0.17
(1,54)	1:269:A:GLY:H	1:267:A:PRO:HD2	14	0.22	0.05	0.21

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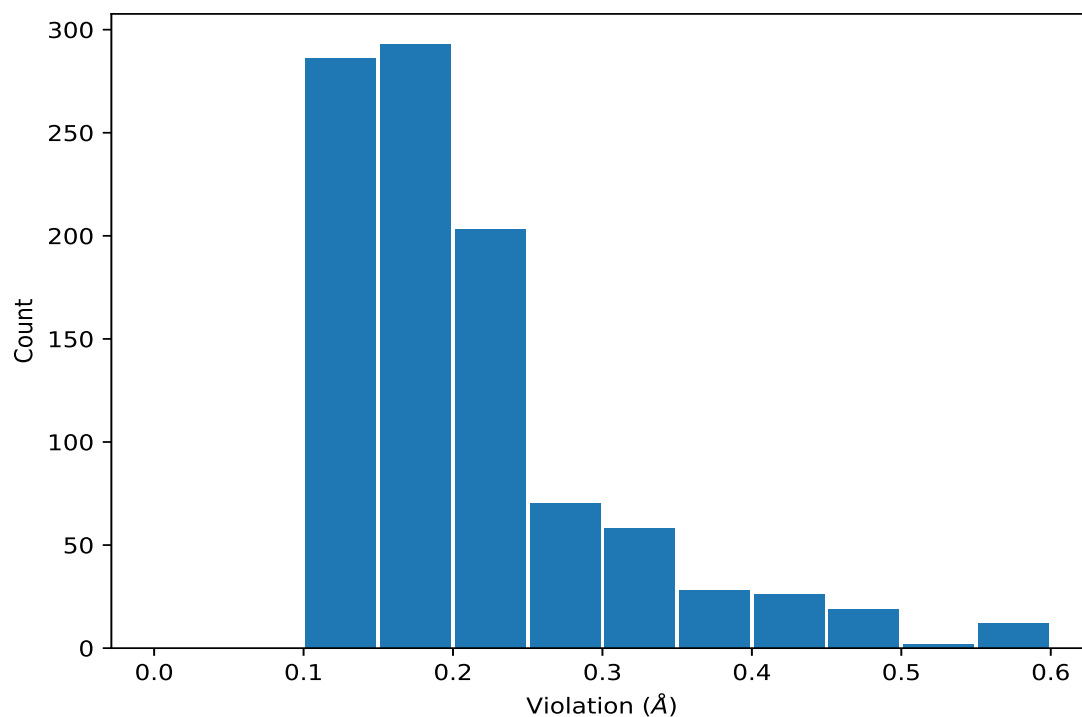
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,54)	1:269:A:GLY:H	1:267:A:PRO:HD3	14	0.22	0.05	0.21
(1,179)	2:255:B:LEU:H	2:252:B:SER:HA	14	0.17	0.04	0.18
(1,102)	1:278:A:ILE:H	1:275:A:ILE:HA	14	0.15	0.02	0.15

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table 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)
(1,37)	1:263:A:ALA:HB1	1:267:A:PRO:HB2	11	0.57
(1,37)	1:263:A:ALA:HB1	1:267:A:PRO:HB3	11	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:263:A:ALA:HB2	1:267:A:PRO:HB2	11	0.57
(1,37)	1:263:A:ALA:HB2	1:267:A:PRO:HB3	11	0.57
(1,37)	1:263:A:ALA:HB3	1:267:A:PRO:HB2	11	0.57
(1,37)	1:263:A:ALA:HB3	1:267:A:PRO:HB3	11	0.57
(1,37)	1:263:A:ALA:HB1	1:267:A:PRO:HB2	6	0.56
(1,37)	1:263:A:ALA:HB1	1:267:A:PRO:HB3	6	0.56
(1,37)	1:263:A:ALA:HB2	1:267:A:PRO:HB2	6	0.56
(1,37)	1:263:A:ALA:HB2	1:267:A:PRO:HB3	6	0.56
(1,37)	1:263:A:ALA:HB3	1:267:A:PRO:HB2	6	0.56
(1,37)	1:263:A:ALA:HB3	1:267:A:PRO:HB3	6	0.56
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	3	0.51
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	11	0.51
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	4	0.49
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	5	0.49
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	7	0.49
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	10	0.49
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	12	0.49
(1,243)	2:265:B:LYS:H	2:264:B:TRP:HA	13	0.49

10 Dihedral-angle violation analysis [i](#)

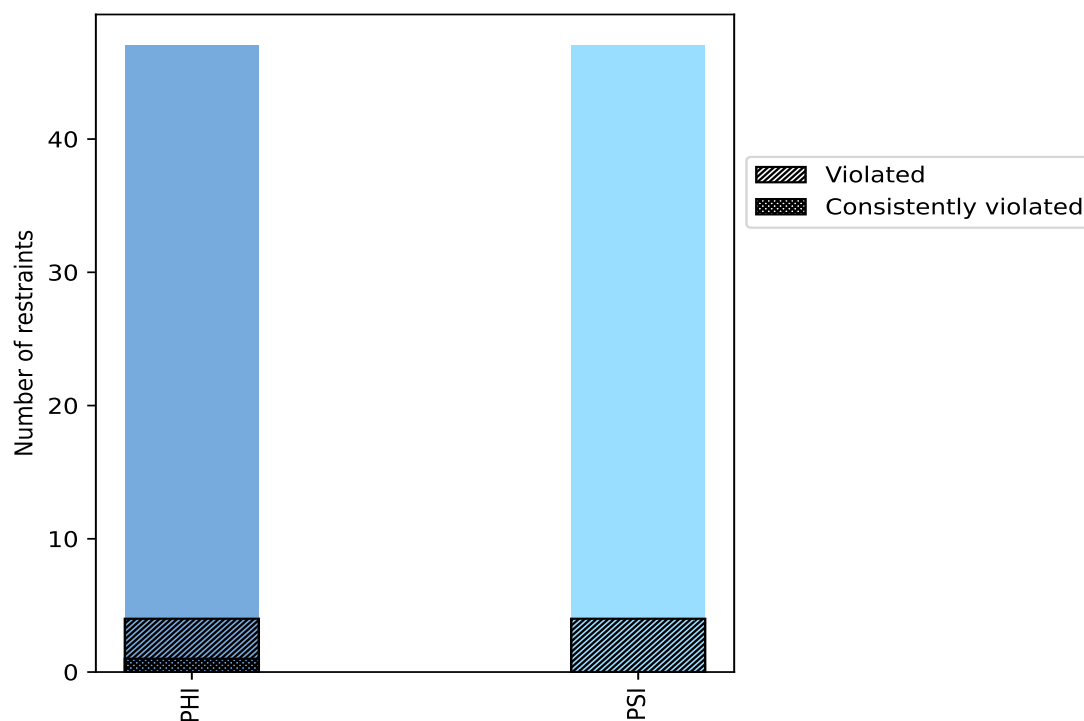
10.1 Summary of dihedral-angle violations [i](#)

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	47	50.0	4	8.5	4.3	1	2.1	1.1
PSI	47	50.0	4	8.5	4.3	0	0.0	0.0
Total	94	100.0	8	8.5	8.5	1	1.1	1.1

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 [i](#)



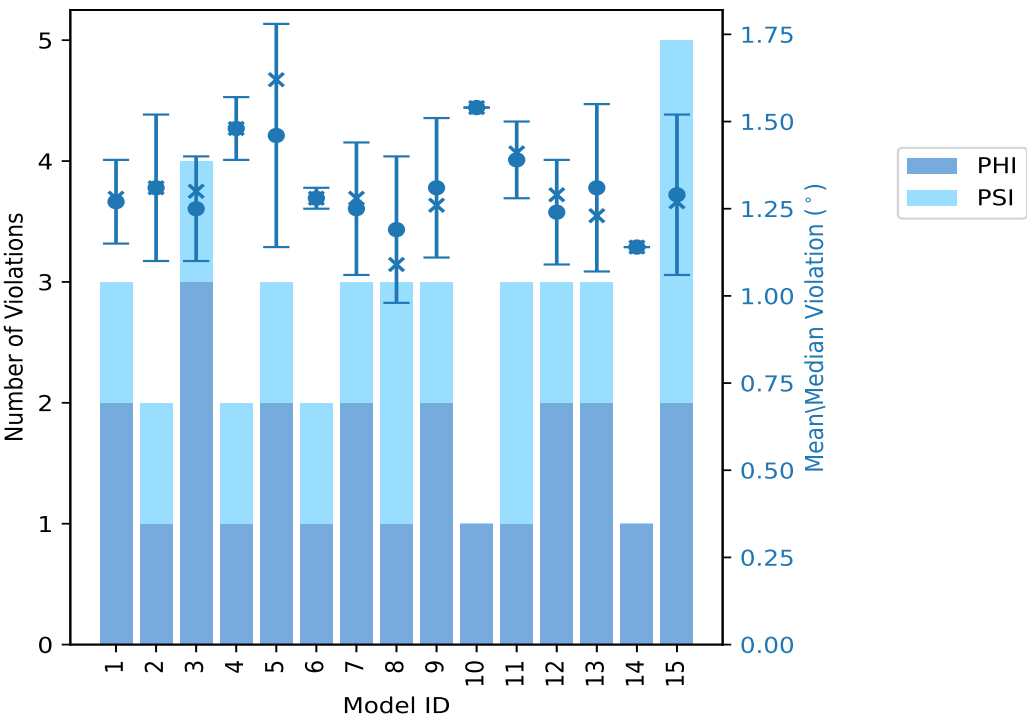
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	PSI	Total				
1	2	1	3	1.27	1.41	0.12	1.28
2	1	1	2	1.31	1.52	0.21	1.31
3	3	1	4	1.25	1.41	0.15	1.3
4	1	1	2	1.48	1.56	0.09	1.48
5	2	1	3	1.46	1.75	0.32	1.62
6	1	1	2	1.28	1.31	0.03	1.28
7	2	1	3	1.25	1.47	0.19	1.28
8	1	2	3	1.19	1.48	0.21	1.09
9	2	1	3	1.31	1.57	0.2	1.26
10	1	0	1	1.54	1.54	0.0	1.54
11	1	2	3	1.39	1.52	0.11	1.41
12	2	1	3	1.24	1.39	0.15	1.29
13	2	1	3	1.31	1.63	0.24	1.23
14	1	0	1	1.14	1.14	0.0	1.14
15	2	3	5	1.29	1.67	0.23	1.27

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

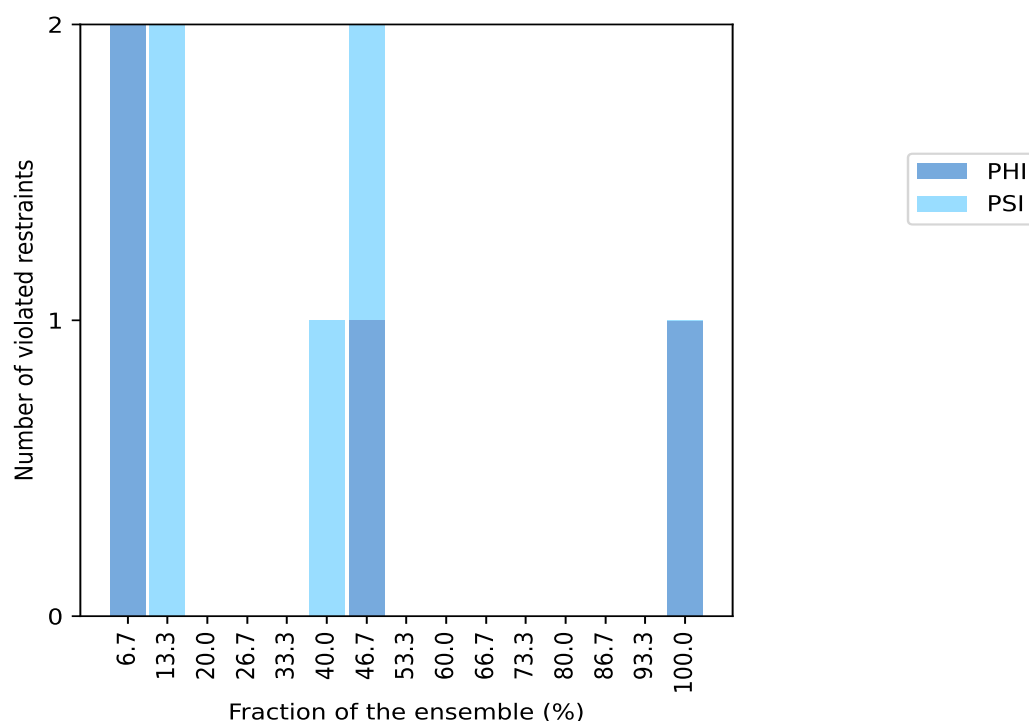
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	PSI	Total	Count ¹	%
2	0	2	1	6.7
0	2	2	2	13.3
0	0	0	3	20.0
0	0	0	4	26.7
0	0	0	5	33.3
0	1	1	6	40.0
1	1	2	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
1	0	1	15	100.0

¹ Number of models with violations

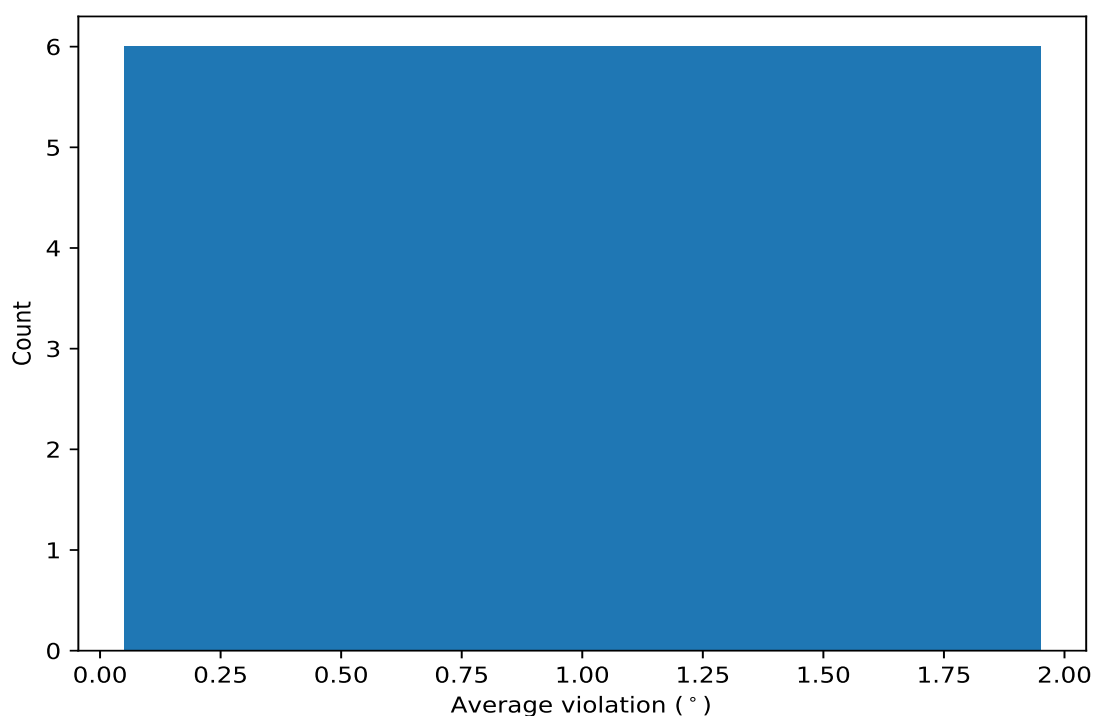
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

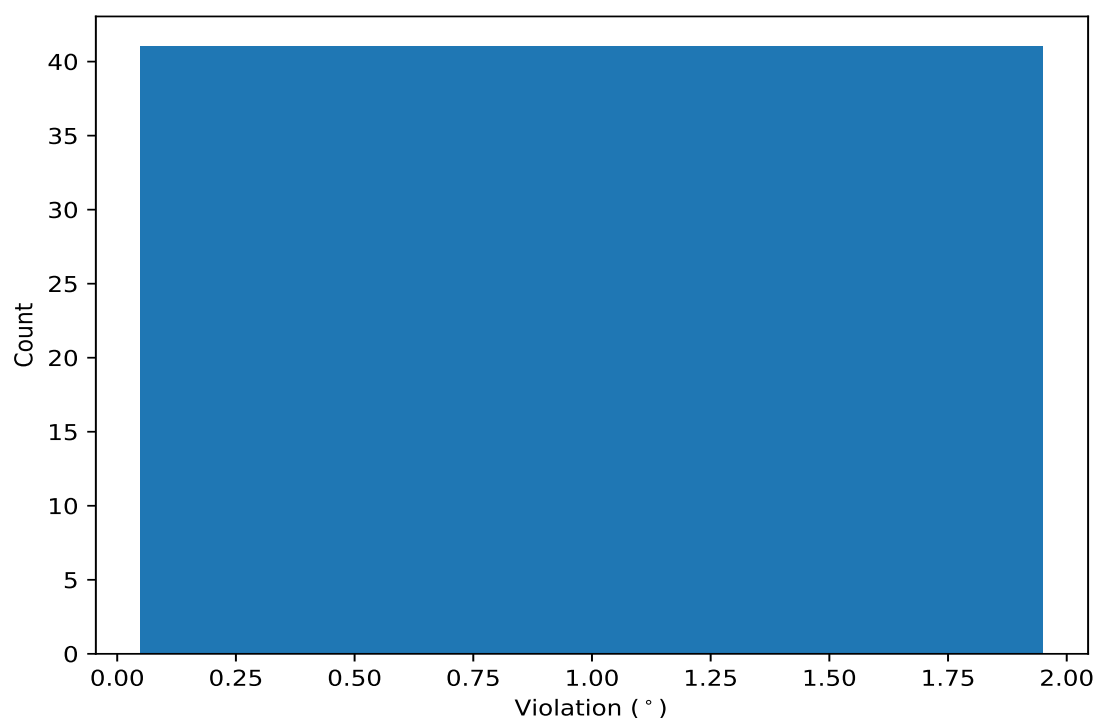
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	15	1.43	0.13	1.41
(1,11)	1:263:A:ALA:C	1:264:A:VAL:N	1:264:A:VAL:CA	1:264:A:VAL:C	7	1.41	0.24	1.32
(1,4)	1:258:A:LEU:N	1:258:A:LEU:CA	1:258:A:LEU:C	1:259:A:PHE:N	7	1.17	0.13	1.1
(1,16)	1:267:A:PRO:N	1:267:A:PRO:CA	1:267:A:PRO:C	1:268:A:VAL:N	6	1.16	0.11	1.17
(1,10)	1:263:A:ALA:N	1:263:A:ALA:CA	1:263:A:ALA:C	1:264:A:VAL:N	2	1.27	0.26	1.27
(1,18)	1:268:A:VAL:N	1:268:A:VAL:CA	1:268:A:VAL:C	1:269:A:GLY:N	2	1.18	0.09	1.18

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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 [i](#)

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 (°)
(1,11)	1:263:A:ALA:C	1:264:A:VAL:N	1:264:A:VAL:CA	1:264:A:VAL:C	5	1.75
(1,11)	1:263:A:ALA:C	1:264:A:VAL:N	1:264:A:VAL:CA	1:264:A:VAL:C	15	1.67
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	13	1.63
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	5	1.62
(1,11)	1:263:A:ALA:C	1:264:A:VAL:N	1:264:A:VAL:CA	1:264:A:VAL:C	9	1.57
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	4	1.56
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	10	1.54
(1,10)	1:263:A:ALA:N	1:263:A:ALA:CA	1:263:A:ALA:C	1:264:A:VAL:N	11	1.52
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	2	1.52
(1,5)	1:258:A:LEU:C	1:259:A:PHE:N	1:259:A:PHE:CA	1:259:A:PHE:C	8	1.48