



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 08:49 PM EDT

PDB ID : 2LX0  
BMRB ID : 18655  
Title : Arced helix (ArcH) NMR structure of the reovirus p14 fusion-associated small transmembrane (FAST) protein transmembrane domain (TMD) in dodecyl phosphocholine (DPC) micelles  
Authors : Sarker, M.; Key, T.; Duncan, R.; Rainey, J.K.  
Deposited on : 2012-08-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) 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

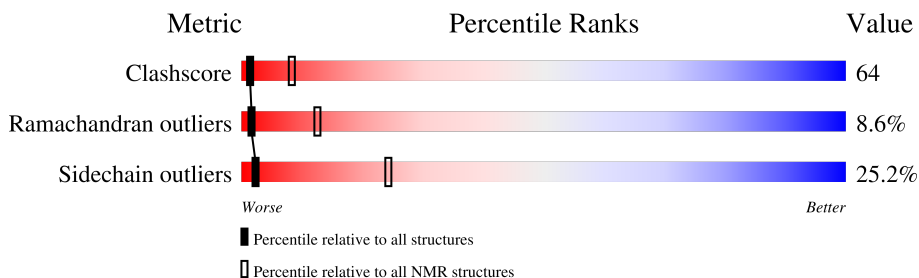
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 57%.

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  $\geq 3$ , 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	32	

## 2 Ensemble composition and analysis i

This entry contains 50 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:31 (28)	0.38	10

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 7 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 10, 11, 13, 20, 22, 23, 25, 28, 32, 33, 34, 36, 37, 40, 47
2	4, 9, 15, 21, 24, 27, 38, 43, 44
3	5, 7, 8, 12, 14, 17, 39, 50
4	19, 29, 30, 31
5	35, 41
6	16, 18
7	42, 48
Single-model clusters	26; 45; 46; 49

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 567 atoms, of which 294 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Membrane fusion protein p14.

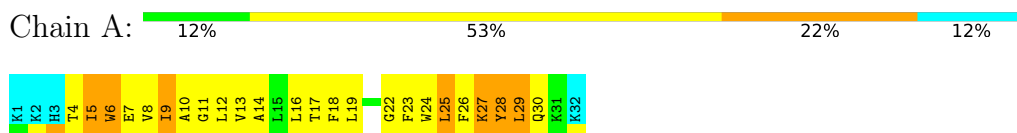
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	32	567	192	294	42	39	0

## 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: Membrane fusion protein p14

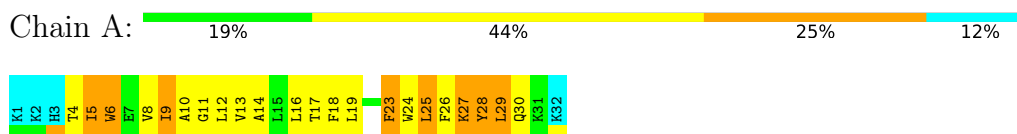


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

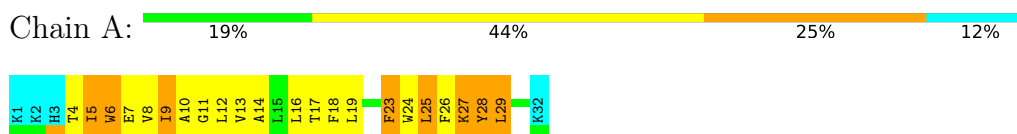
#### 4.2.1 Score per residue for model 1

- Molecule 1: Membrane fusion protein p14



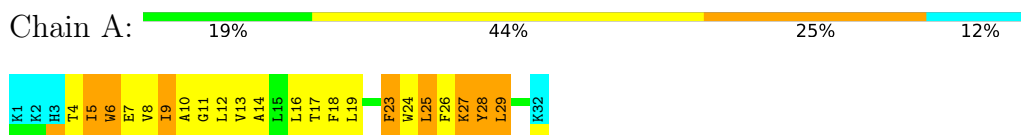
#### 4.2.2 Score per residue for model 2

- Molecule 1: Membrane fusion protein p14



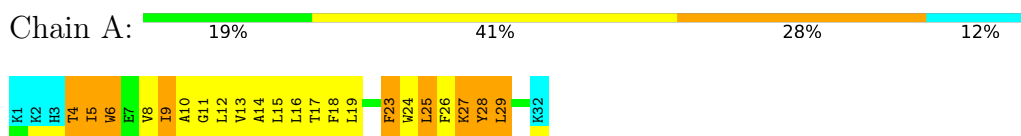
### 4.2.3 Score per residue for model 3

- Molecule 1: Membrane fusion protein p14



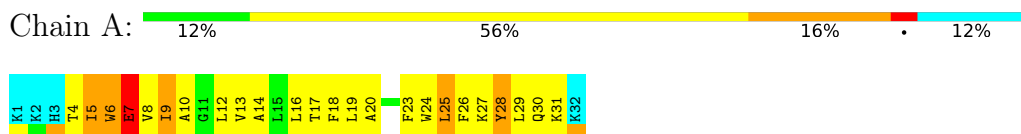
### 4.2.4 Score per residue for model 4

- Molecule 1: Membrane fusion protein p14



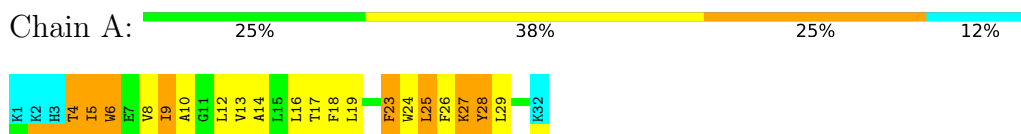
### 4.2.5 Score per residue for model 5

- Molecule 1: Membrane fusion protein p14



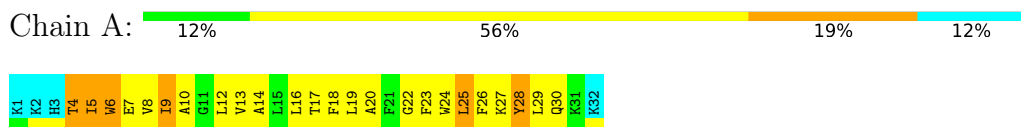
### 4.2.6 Score per residue for model 6

- Molecule 1: Membrane fusion protein p14



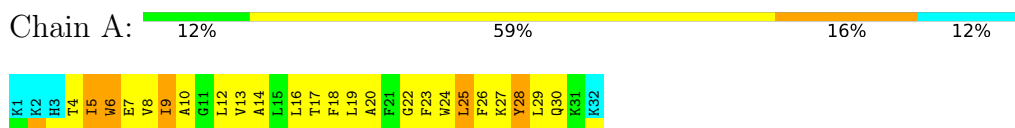
### 4.2.7 Score per residue for model 7

- Molecule 1: Membrane fusion protein p14



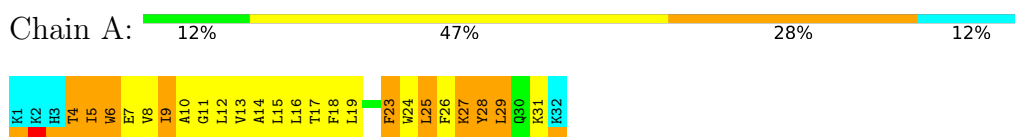
#### 4.2.8 Score per residue for model 8

- Molecule 1: Membrane fusion protein p14



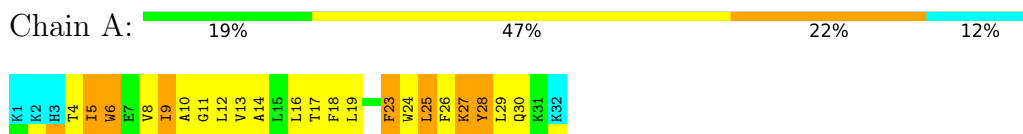
#### 4.2.9 Score per residue for model 9

- Molecule 1: Membrane fusion protein p14



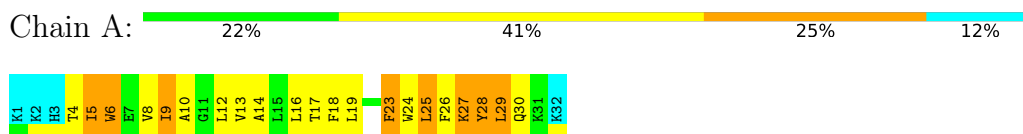
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Membrane fusion protein p14



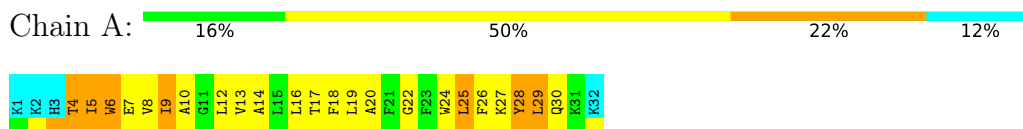
#### 4.2.11 Score per residue for model 11

- Molecule 1: Membrane fusion protein p14



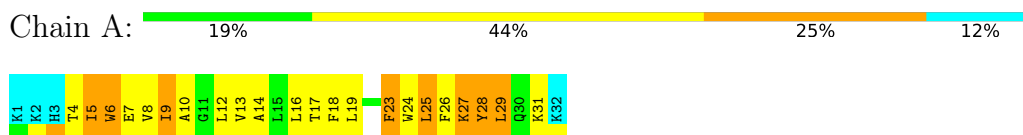
#### 4.2.12 Score per residue for model 12

- Molecule 1: Membrane fusion protein p14



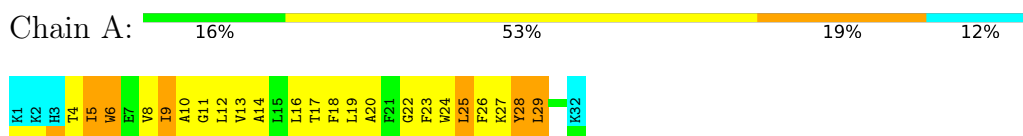
### 4.2.13 Score per residue for model 13

- Molecule 1: Membrane fusion protein p14



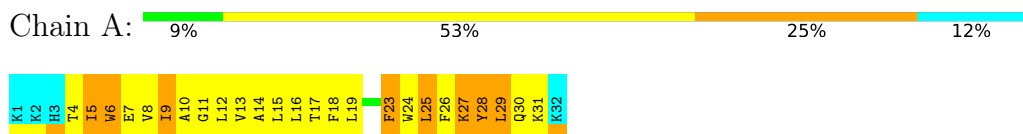
### 4.2.14 Score per residue for model 14

- Molecule 1: Membrane fusion protein p14



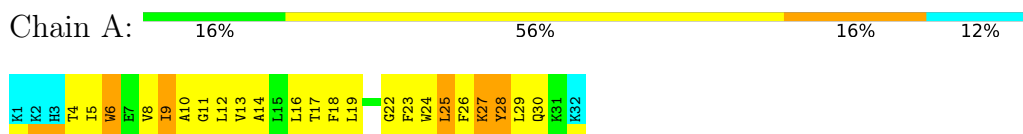
### 4.2.15 Score per residue for model 15

- Molecule 1: Membrane fusion protein p14



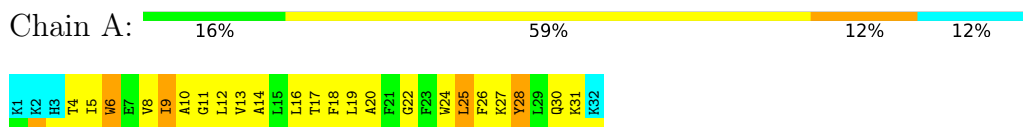
### 4.2.16 Score per residue for model 16

- Molecule 1: Membrane fusion protein p14



### 4.2.17 Score per residue for model 17

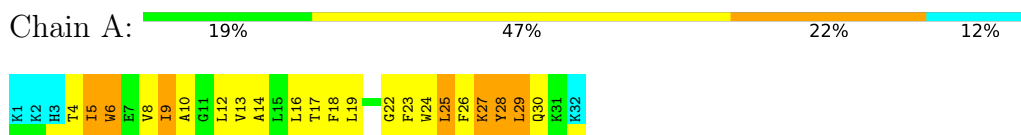
- Molecule 1: Membrane fusion protein p14





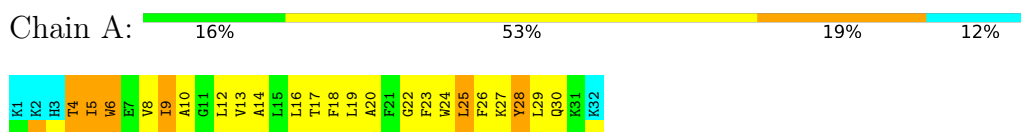
#### 4.2.18 Score per residue for model 18

- Molecule 1: Membrane fusion protein p14



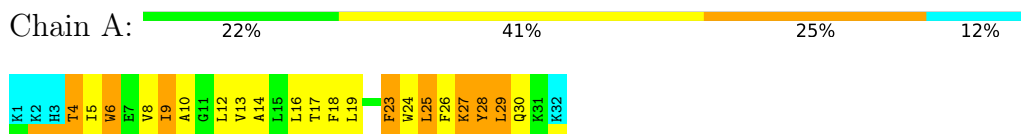
#### 4.2.19 Score per residue for model 19

- Molecule 1: Membrane fusion protein p14



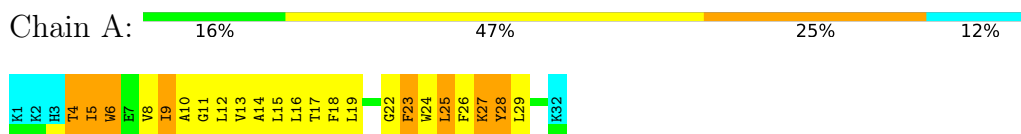
#### 4.2.20 Score per residue for model 20

- Molecule 1: Membrane fusion protein p14



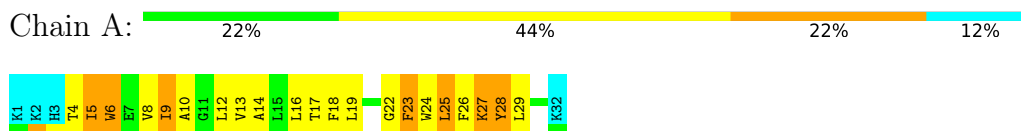
#### 4.2.21 Score per residue for model 21

- Molecule 1: Membrane fusion protein p14



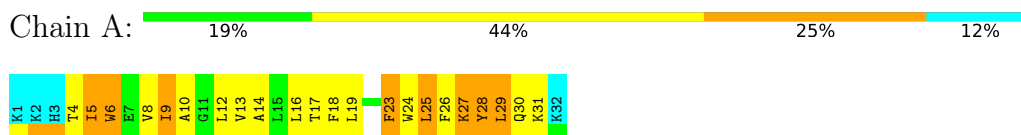
#### 4.2.22 Score per residue for model 22

- Molecule 1: Membrane fusion protein p14



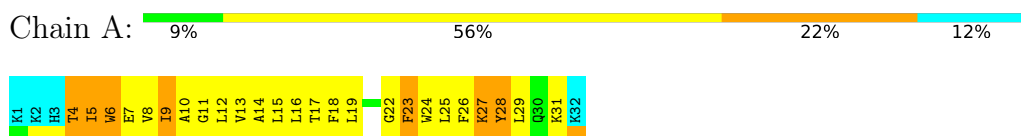
#### 4.2.23 Score per residue for model 23

- Molecule 1: Membrane fusion protein p14



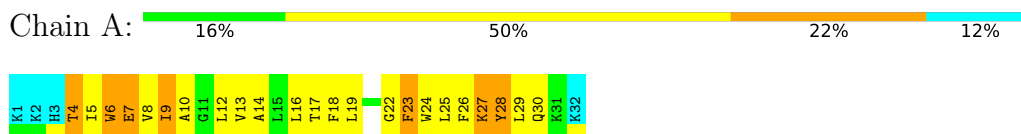
#### 4.2.24 Score per residue for model 24

- Molecule 1: Membrane fusion protein p14



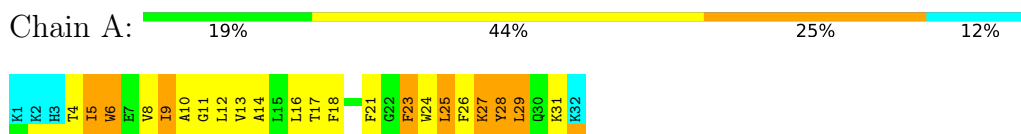
#### 4.2.25 Score per residue for model 25

- Molecule 1: Membrane fusion protein p14



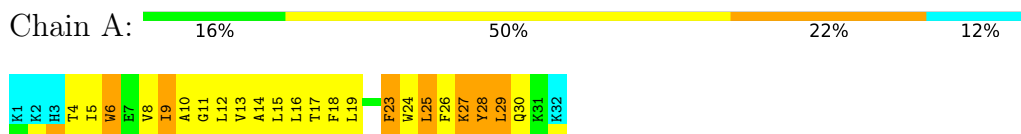
#### 4.2.26 Score per residue for model 26

- Molecule 1: Membrane fusion protein p14



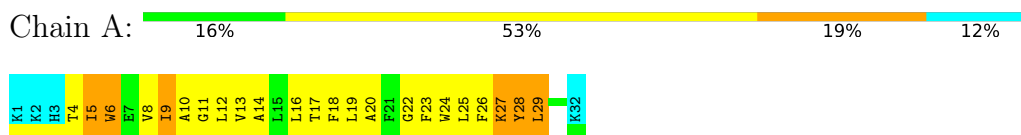
#### 4.2.27 Score per residue for model 27

- Molecule 1: Membrane fusion protein p14



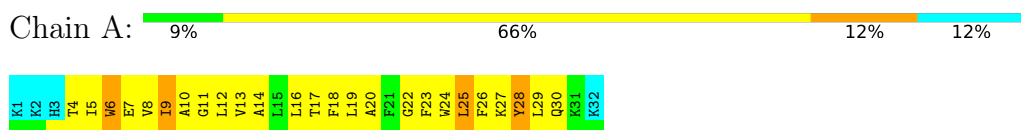
#### 4.2.28 Score per residue for model 28

- Molecule 1: Membrane fusion protein p14



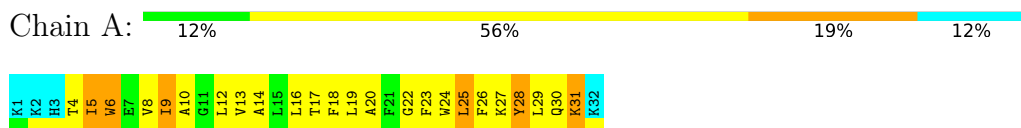
#### 4.2.29 Score per residue for model 29

- Molecule 1: Membrane fusion protein p14



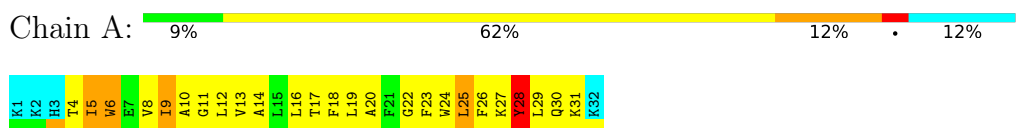
#### 4.2.30 Score per residue for model 30

- Molecule 1: Membrane fusion protein p14



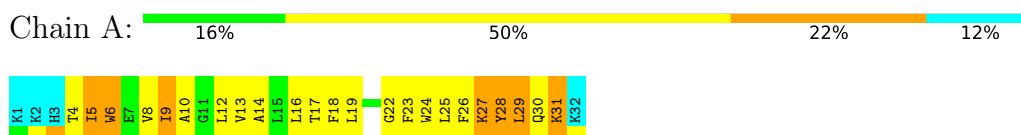
#### 4.2.31 Score per residue for model 31

- Molecule 1: Membrane fusion protein p14



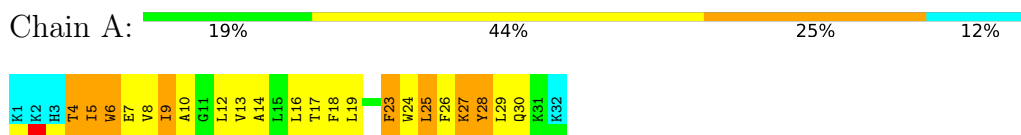
#### 4.2.32 Score per residue for model 32

- Molecule 1: Membrane fusion protein p14



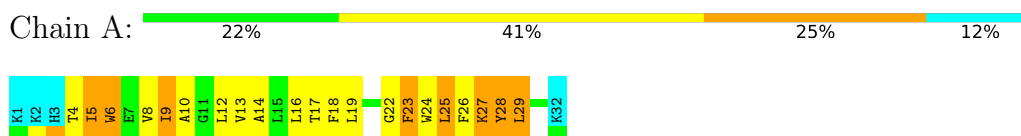
### 4.2.33 Score per residue for model 33

- Molecule 1: Membrane fusion protein p14



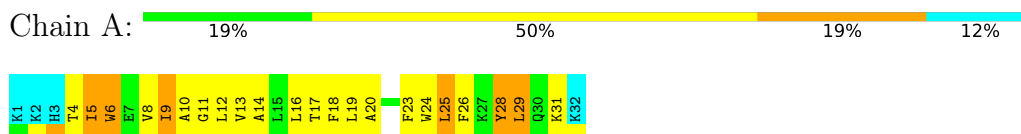
### 4.2.34 Score per residue for model 34

- Molecule 1: Membrane fusion protein p14



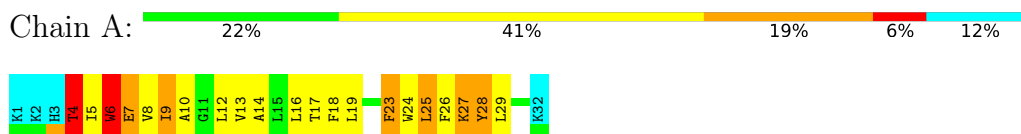
### 4.2.35 Score per residue for model 35

- Molecule 1: Membrane fusion protein p14



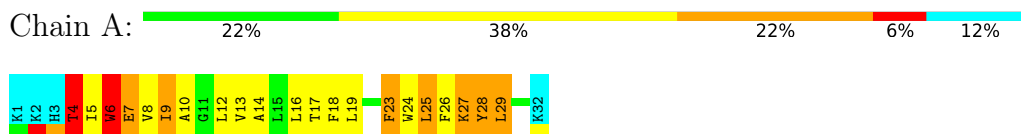
### 4.2.36 Score per residue for model 36

- Molecule 1: Membrane fusion protein p14



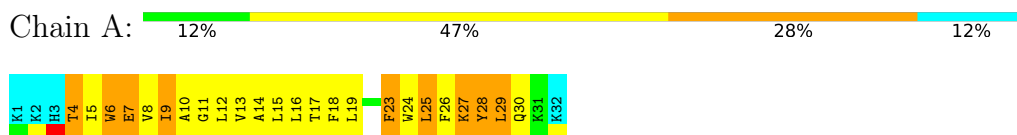
### 4.2.37 Score per residue for model 37

- Molecule 1: Membrane fusion protein p14



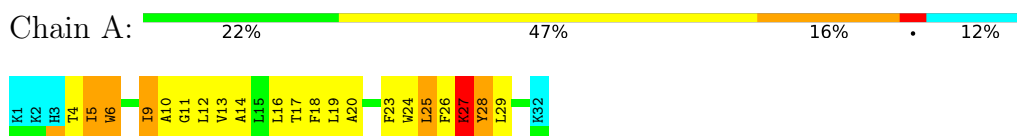
#### 4.2.38 Score per residue for model 38

- Molecule 1: Membrane fusion protein p14



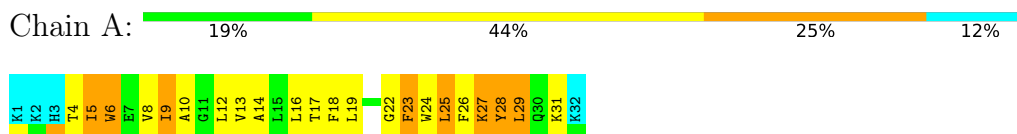
#### 4.2.39 Score per residue for model 39

- Molecule 1: Membrane fusion protein p14



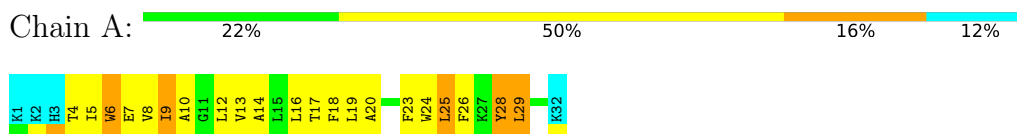
#### 4.2.40 Score per residue for model 40

- Molecule 1: Membrane fusion protein p14



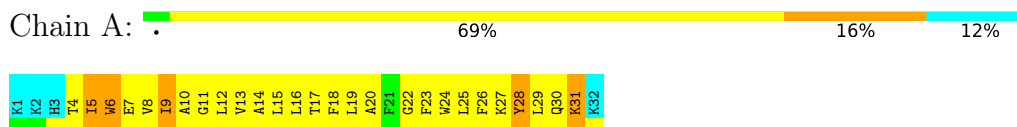
#### 4.2.41 Score per residue for model 41

- Molecule 1: Membrane fusion protein p14



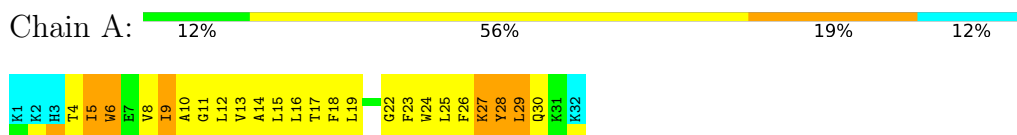
#### 4.2.42 Score per residue for model 42

- Molecule 1: Membrane fusion protein p14



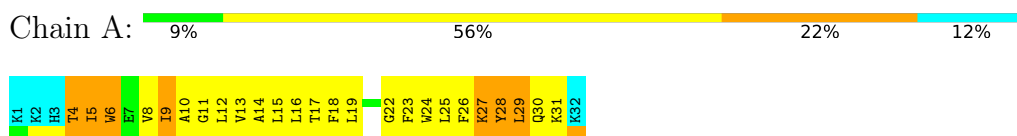
#### 4.2.43 Score per residue for model 43

- Molecule 1: Membrane fusion protein p14



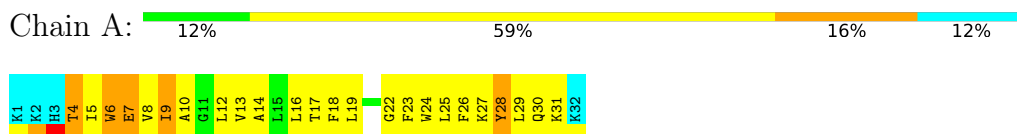
#### 4.2.44 Score per residue for model 44

- Molecule 1: Membrane fusion protein p14



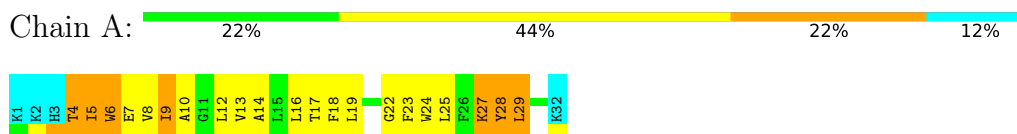
#### 4.2.45 Score per residue for model 45

- Molecule 1: Membrane fusion protein p14



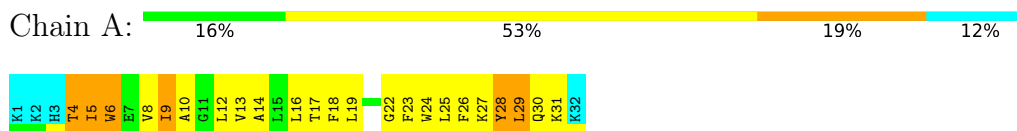
#### 4.2.46 Score per residue for model 46

- Molecule 1: Membrane fusion protein p14



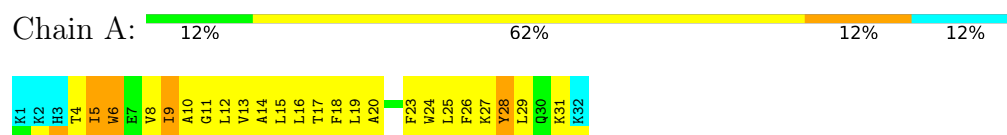
#### 4.2.47 Score per residue for model 47

- Molecule 1: Membrane fusion protein p14



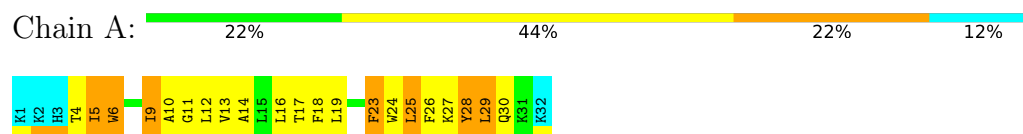
#### 4.2.48 Score per residue for model 48

- Molecule 1: Membrane fusion protein p14



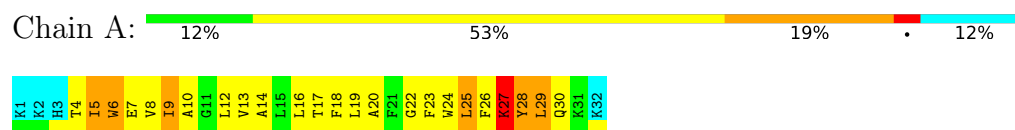
#### 4.2.49 Score per residue for model 49

- Molecule 1: Membrane fusion protein p14



#### 4.2.50 Score per residue for model 50

- Molecule 1: Membrane fusion protein p14



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 50 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	structure solution	2.18
X-PLOR NIH	refinement	2.18

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	287
Number of shifts mapped to atoms	286
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	57%



## 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	235	246	246	31±3
All	All	11750	12300	12300	1550

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 64.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:GLY:O	1:A:15:LEU:HD12	0.67	1.90	42	11
1:A:29:LEU:HD12	1:A:29:LEU:O	0.64	1.92	43	2
1:A:24:TRP:CZ2	1:A:28:TYR:CD2	0.62	2.88	46	20
1:A:24:TRP:CZ2	1:A:28:TYR:CE2	0.62	2.87	12	16
1:A:4:THR:HG23	1:A:5:ILE:N	0.61	2.09	19	46
1:A:29:LEU:C	1:A:29:LEU:HD12	0.60	2.17	47	1
1:A:29:LEU:HD12	1:A:29:LEU:C	0.60	2.17	43	1
1:A:24:TRP:CE2	1:A:28:TYR:CD2	0.59	2.90	14	19
1:A:6:TRP:O	1:A:10:ALA:N	0.58	2.36	20	50
1:A:4:THR:HG23	1:A:5:ILE:H	0.58	1.59	11	44
1:A:29:LEU:O	1:A:29:LEU:HD23	0.57	2.00	7	25
1:A:26:PHE:O	1:A:30:GLN:N	0.56	2.38	49	17
1:A:22:GLY:O	1:A:26:PHE:CD2	0.55	2.60	16	17
1:A:10:ALA:O	1:A:14:ALA:N	0.54	2.40	49	50

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ALA:O	1:A:18:PHE:N	0.54	2.40	40	50
1:A:13:VAL:O	1:A:16:LEU:N	0.54	2.40	49	50
1:A:4:THR:OG1	1:A:5:ILE:N	0.54	2.41	38	50
1:A:19:LEU:HD22	1:A:19:LEU:N	0.54	2.17	39	6
1:A:4:THR:HG23	1:A:6:TRP:H	0.54	1.62	19	13
1:A:13:VAL:O	1:A:17:THR:N	0.54	2.41	14	50
1:A:19:LEU:N	1:A:19:LEU:CD2	0.54	2.71	46	48
1:A:19:LEU:N	1:A:19:LEU:HD22	0.53	2.19	46	42
1:A:9:ILE:O	1:A:13:VAL:N	0.53	2.42	37	50
1:A:26:PHE:O	1:A:28:TYR:N	0.53	2.42	44	41
1:A:23:PHE:CG	1:A:23:PHE:O	0.52	2.62	35	4
1:A:23:PHE:O	1:A:23:PHE:CG	0.52	2.63	46	3
1:A:9:ILE:O	1:A:13:VAL:HG23	0.52	2.04	27	41
1:A:24:TRP:O	1:A:27:LYS:N	0.51	2.42	46	1
1:A:6:TRP:O	1:A:8:VAL:N	0.51	2.43	25	21
1:A:10:ALA:C	1:A:12:LEU:N	0.51	2.64	27	50
1:A:26:PHE:C	1:A:28:TYR:H	0.51	2.08	16	44
1:A:10:ALA:O	1:A:13:VAL:N	0.50	2.45	41	50
1:A:17:THR:O	1:A:20:ALA:N	0.50	2.44	12	17
1:A:5:ILE:O	1:A:8:VAL:N	0.50	2.44	24	46
1:A:24:TRP:O	1:A:25:LEU:C	0.50	2.50	33	50
1:A:19:LEU:CD1	1:A:19:LEU:N	0.50	2.74	40	1
1:A:4:THR:CG2	1:A:5:ILE:N	0.50	2.74	19	21
1:A:27:LYS:CD	1:A:27:LYS:N	0.50	2.75	18	6
1:A:28:TYR:CD1	1:A:28:TYR:C	0.49	2.85	47	31
1:A:30:GLN:CG	1:A:30:GLN:O	0.49	2.60	32	9
1:A:29:LEU:O	1:A:29:LEU:HD13	0.49	2.08	40	2
1:A:24:TRP:NE1	1:A:28:TYR:CG	0.48	2.81	17	1
1:A:4:THR:CG2	1:A:5:ILE:H	0.48	2.20	29	42
1:A:19:LEU:N	1:A:19:LEU:HD12	0.48	2.24	40	1
1:A:6:TRP:C	1:A:8:VAL:N	0.48	2.67	25	26
1:A:12:LEU:O	1:A:16:LEU:CD1	0.48	2.62	26	46
1:A:23:PHE:O	1:A:27:LYS:CG	0.48	2.62	15	26
1:A:26:PHE:C	1:A:28:TYR:N	0.47	2.68	23	39
1:A:6:TRP:O	1:A:11:GLY:N	0.47	2.47	27	19
1:A:12:LEU:O	1:A:16:LEU:HD12	0.47	2.09	17	33
1:A:28:TYR:C	1:A:28:TYR:CD1	0.47	2.84	43	1
1:A:25:LEU:O	1:A:29:LEU:N	0.47	2.43	34	4
1:A:28:TYR:CG	1:A:29:LEU:N	0.46	2.83	46	10
1:A:29:LEU:C	1:A:29:LEU:CD1	0.46	2.83	47	2
1:A:7:GLU:N	1:A:7:GLU:OE1	0.45	2.50	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:PHE:O	1:A:30:GLN:CB	0.45	2.64	49	1
1:A:28:TYR:O	1:A:28:TYR:CD1	0.45	2.70	21	4
1:A:10:ALA:O	1:A:12:LEU:N	0.44	2.51	27	50
1:A:6:TRP:CG	1:A:10:ALA:CB	0.44	3.00	4	43
1:A:30:GLN:O	1:A:30:GLN:CG	0.44	2.65	16	4
1:A:24:TRP:O	1:A:28:TYR:N	0.44	2.49	49	1
1:A:25:LEU:O	1:A:29:LEU:CB	0.44	2.66	33	10
1:A:22:GLY:C	1:A:24:TRP:N	0.43	2.69	40	7
1:A:18:PHE:O	1:A:22:GLY:N	0.43	2.47	25	6
1:A:24:TRP:NE1	1:A:28:TYR:CB	0.43	2.82	17	1
1:A:10:ALA:C	1:A:12:LEU:H	0.42	2.18	49	36
1:A:6:TRP:C	1:A:8:VAL:H	0.42	2.17	29	8
1:A:27:LYS:CD	1:A:27:LYS:H	0.42	2.25	50	1
1:A:5:ILE:O	1:A:6:TRP:C	0.42	2.58	37	5
1:A:9:ILE:O	1:A:13:VAL:CG2	0.42	2.68	27	1
1:A:7:GLU:N	1:A:7:GLU:CD	0.41	2.73	25	1
1:A:21:PHE:CD1	1:A:21:PHE:N	0.41	2.89	26	1
1:A:28:TYR:CD1	1:A:28:TYR:O	0.41	2.74	49	1
1:A:17:THR:HG22	1:A:18:PHE:N	0.41	2.31	28	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	28/32 (88%)	17±1 (62±4%)	8±1 (29±4%)	2±1 (9±4%)	2	12
All	All	1400/1600 (88%)	869 (62%)	410 (29%)	121 (9%)	2	12

All 6 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	27	LYS	46
1	A	25	LEU	39
1	A	4	THR	18

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Mol	Chain	Res	Type	Models (Total)
1	A	7	GLU	15
1	A	6	TRP	2
1	A	28	TYR	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	23/27 (85%)	17±1 (75±4%)	6±1 (25±4%)	2	24
All	All	1150/1350 (85%)	860 (75%)	290 (25%)	2	24

All 10 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	6	TRP	50
1	A	9	ILE	50
1	A	28	TYR	50
1	A	23	PHE	41
1	A	5	ILE	39
1	A	29	LEU	36
1	A	31	LYS	12
1	A	7	GLU	7
1	A	27	LYS	3
1	A	4	THR	2

### 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 57% for the well-defined parts and 56% 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 [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	287
Number of shifts mapped to atoms	286
Number of unparsed shifts	0
Number of shifts with mapping errors	1
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. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	HIS	HD1	11.126	0.003	1

#### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

#### 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 57%, i.e. 244 atoms were assigned a chemical shift out of a possible 427. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	66/142 (46%)	58/58 (100%)	0/56 (0%)	8/28 (29%)
Sidechain	142/212 (67%)	142/143 (99%)	0/66 (0%)	0/3 (0%)
Aromatic	36/73 (49%)	36/36 (100%)	0/35 (0%)	0/2 (0%)
Overall	244/427 (57%)	236/237 (100%)	0/157 (0%)	8/33 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 278 atoms were assigned a chemical shift out of a possible 496. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	71/162 (44%)	63/66 (95%)	0/64 (0%)	8/32 (25%)
Sidechain	168/254 (66%)	168/169 (99%)	0/79 (0%)	0/6 (0%)
Aromatic	39/80 (49%)	39/40 (98%)	0/37 (0%)	0/3 (0%)
Overall	278/496 (56%)	270/275 (98%)	0/180 (0%)	8/41 (20%)

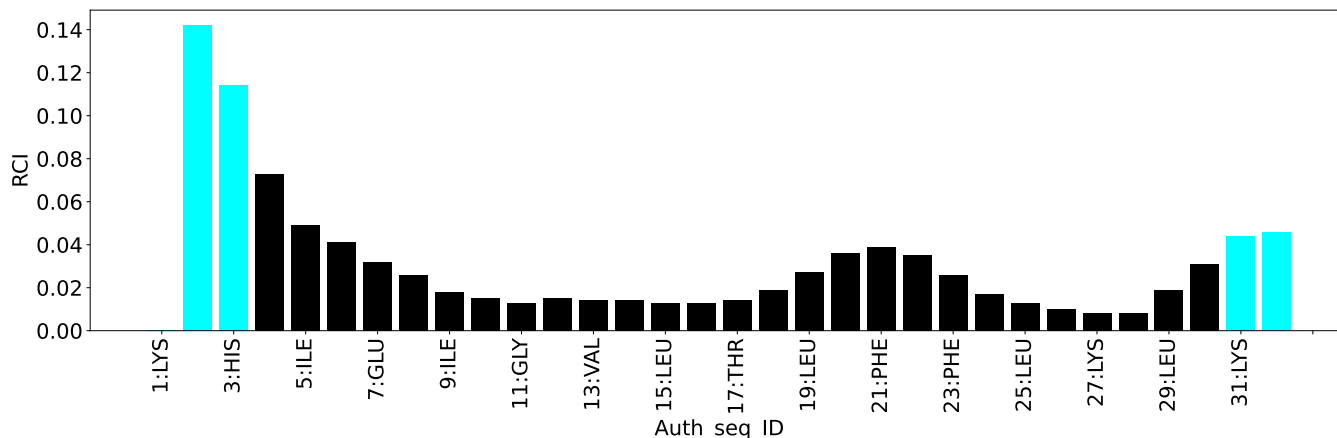
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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:



## 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	1887
Intra-residue ( $ i-j =0$ )	739
Sequential ( $ i-j =1$ )	496
Medium range ( $ i-j >1$ and $ i-j <5$ )	621
Long range ( $ i-j \geq 5$ )	11
Inter-chain	0
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	38
Number of unmapped restraints	0
Number of restraints per residue	60.2
Number of long range restraints per residue <sup>1</sup>	0.3

<sup>1</sup>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)	1.6	0.2
0.2-0.5 (Medium)	0.5	0.5
>0.5 (Large)	1.5	1.62



### 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)	1.0	8.8
10.0-20.0 (Medium)	0.2	14.2
>20.0 (Large)	None	None

## 9 Distance violation analysis [i](#)

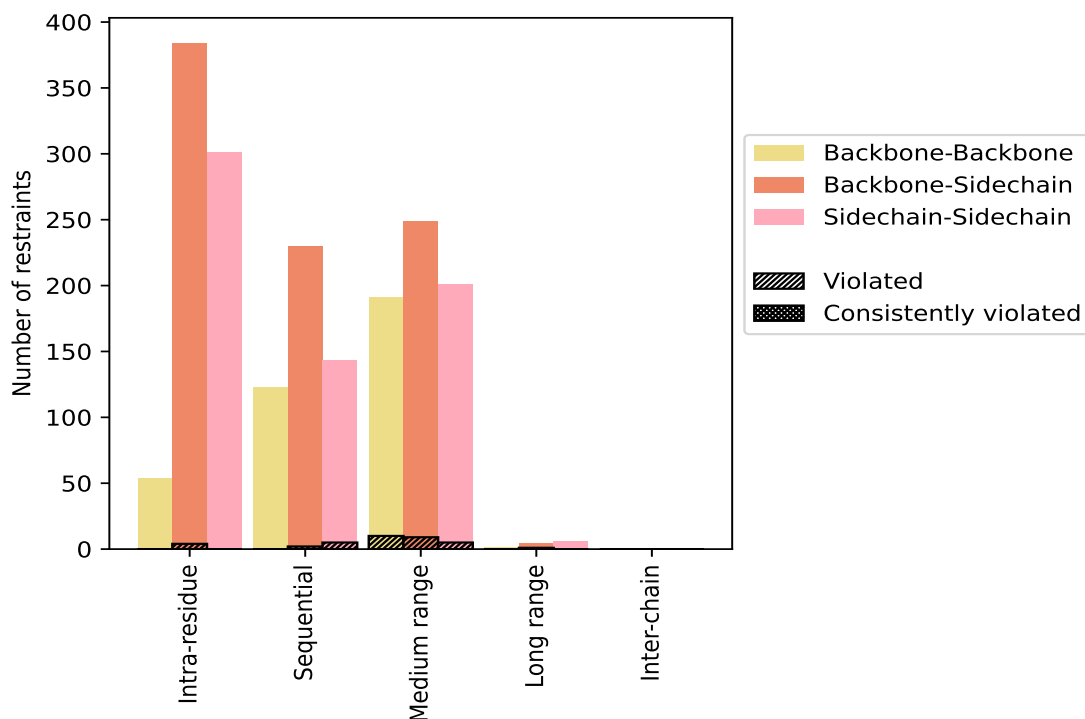
### 9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>739</b>	<b>39.2</b>	<b>4</b>	<b>0.5</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	54	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	384	20.3	4	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	301	16.0	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>496</b>	<b>26.3</b>	<b>7</b>	<b>1.4</b>	<b>0.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	123	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	230	12.2	2	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	143	7.6	5	3.5	0.3	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>621</b>	<b>32.9</b>	<b>16</b>	<b>2.6</b>	<b>0.8</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	171	9.1	2	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	249	13.2	9	3.6	0.5	0	0.0	0.0
Sidechain-Sidechain	201	10.7	5	2.5	0.3	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>11</b>	<b>0.6</b>	<b>1</b>	<b>9.1</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.2	1	25.0	0.1	0	0.0	0.0
Sidechain-Sidechain	6	0.3	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>20</b>	<b>1.1</b>	<b>8</b>	<b>40.0</b>	<b>0.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1887</b>	<b>100.0</b>	<b>36</b>	<b>1.9</b>	<b>1.9</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	369	19.6	10	2.7	0.5	0	0.0	0.0
Backbone-Sidechain	867	45.9	16	1.8	0.8	0	0.0	0.0
Sidechain-Sidechain	651	34.5	10	1.5	0.5	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	0	2	0	0	2	0.87	1.12	0.25	0.87
2	0	0	2	0	0	2	0.87	1.12	0.25	0.87
3	0	0	2	0	0	2	0.9	1.15	0.25	0.9
4	0	0	2	0	0	2	0.88	1.13	0.25	0.88
5	0	0	3	0	0	3	0.54	0.9	0.27	0.48
6	0	0	4	0	0	4	0.5	1.11	0.41	0.38
7	0	0	3	0	0	3	0.31	0.5	0.13	0.23
8	0	0	3	0	0	3	0.4	0.61	0.15	0.3
9	0	0	4	0	0	4	0.49	1.12	0.42	0.37
10	0	1	2	0	0	3	0.63	1.12	0.4	0.62
11	0	1	2	0	0	3	0.64	1.14	0.41	0.64

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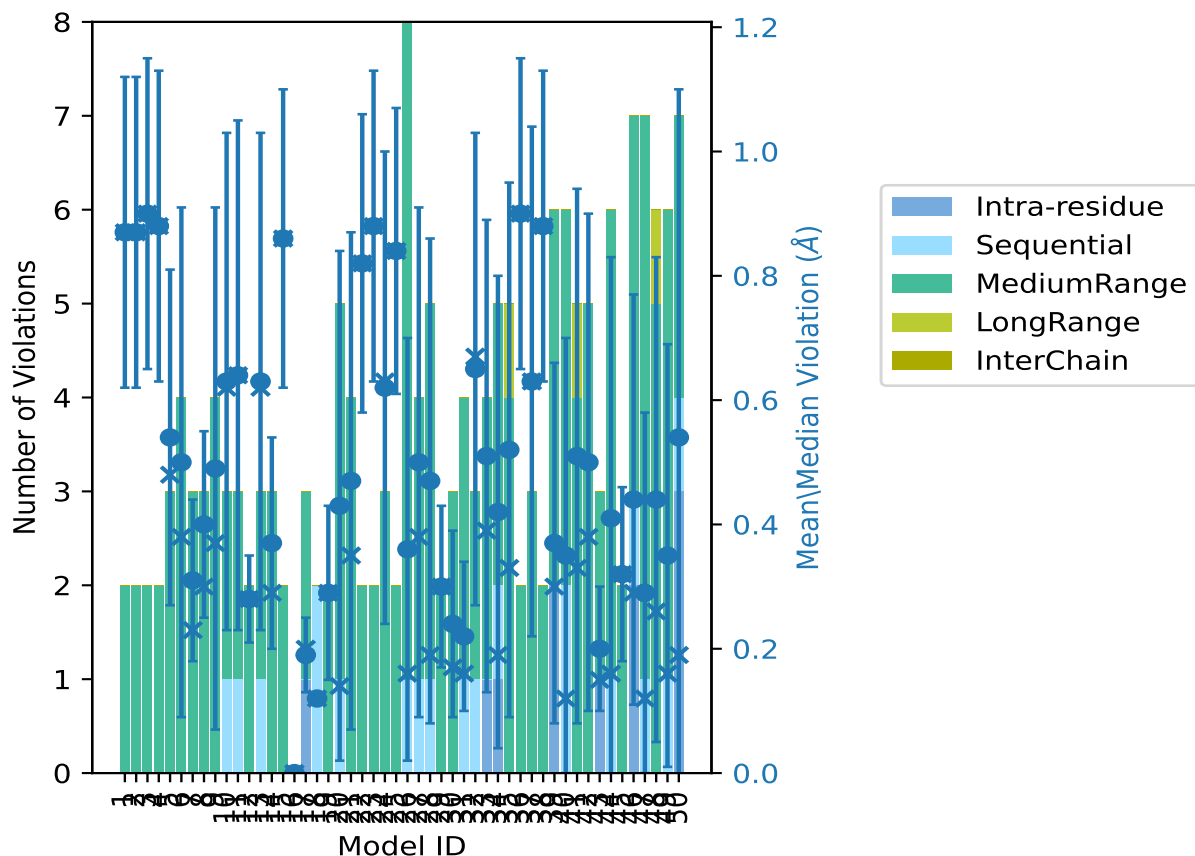
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	0	0	2	0	0	2	0.28	0.34	0.07	0.28
13	0	1	2	0	0	3	0.63	1.12	0.4	0.62
14	0	0	3	0	0	3	0.37	0.61	0.17	0.29
15	0	0	2	0	0	2	0.86	1.1	0.24	0.86
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	1	0	2	0	0	3	0.19	0.26	0.06	0.2
18	0	2	0	0	0	2	0.12	0.12	0.0	0.12
19	0	0	2	0	0	2	0.29	0.43	0.14	0.29
20	0	1	4	0	0	5	0.43	1.14	0.41	0.14
21	0	0	4	0	0	4	0.47	1.07	0.4	0.35
22	0	0	2	0	0	2	0.82	1.06	0.24	0.82
23	0	0	2	0	0	2	0.88	1.13	0.25	0.88
24	0	0	3	0	0	3	0.62	1.09	0.38	0.63
25	0	0	2	0	0	2	0.84	1.06	0.23	0.84
26	0	1	7	0	0	8	0.36	1.13	0.34	0.16
27	0	1	3	0	0	4	0.5	1.12	0.41	0.38
28	0	1	4	0	0	5	0.47	1.12	0.39	0.19
29	0	0	2	0	0	2	0.3	0.43	0.13	0.3
30	0	0	3	0	0	3	0.24	0.45	0.15	0.17
31	0	1	3	0	0	4	0.22	0.43	0.12	0.16
32	0	1	2	0	0	3	0.65	1.1	0.38	0.67
33	1	0	3	0	0	4	0.51	1.1	0.38	0.39
34	1	1	3	0	0	5	0.42	1.08	0.38	0.19
35	0	0	4	1	0	5	0.52	1.25	0.43	0.33
36	0	0	2	0	0	2	0.9	1.16	0.25	0.9
37	0	0	3	0	0	3	0.63	1.13	0.41	0.63
38	0	0	2	0	0	2	0.88	1.13	0.25	0.88
39	2	0	4	0	0	6	0.37	0.93	0.29	0.3
40	0	2	4	0	0	6	0.35	1.04	0.35	0.12
41	0	0	4	1	0	5	0.51	1.22	0.43	0.33
42	0	0	5	0	0	5	0.5	1.15	0.4	0.38
43	1	0	2	0	0	3	0.2	0.35	0.1	0.15
44	0	1	5	0	0	6	0.41	1.19	0.42	0.16
45	0	0	2	0	0	2	0.32	0.45	0.14	0.32
46	2	1	4	0	0	7	0.44	1.12	0.33	0.29
47	0	1	6	0	0	7	0.29	0.89	0.29	0.12
48	0	0	5	1	0	6	0.44	1.17	0.39	0.26
49	0	1	5	0	0	6	0.35	1.02	0.34	0.16
50	3	1	3	0	0	7	0.54	1.62	0.56	0.19

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1839(IR:735, SQ:489, MR:605, LR:10, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
1	5	11	0	0	17	1	2.0
0	1	2	0	0	3	2	4.0
2	0	0	1	0	3	3	6.0
1	0	0	0	0	1	4	8.0
0	0	0	0	0	0	5	10.0
0	0	3	0	0	3	6	12.0

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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	7	14.0
0	0	0	0	0	0	8	16.0
0	0	0	0	0	0	9	18.0
0	0	0	0	0	0	10	20.0
0	0	0	0	0	0	11	22.0
0	1	0	0	0	1	12	24.0
0	0	0	0	0	0	13	26.0
0	0	0	0	0	0	14	28.0
0	0	0	0	0	0	15	30.0
0	0	0	0	0	0	16	32.0
0	0	0	0	0	0	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	0	0	0	20	40.0
0	0	0	0	0	0	21	42.0
0	0	0	0	0	0	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	0	0	0	0	25	50.0
0	0	0	0	0	0	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	0	0	0	0	29	58.0
0	0	0	0	0	0	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	0	0	0	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	0	0	0	0	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0
0	0	0	0	0	0	46	92.0
0	0	0	0	0	0	47	94.0

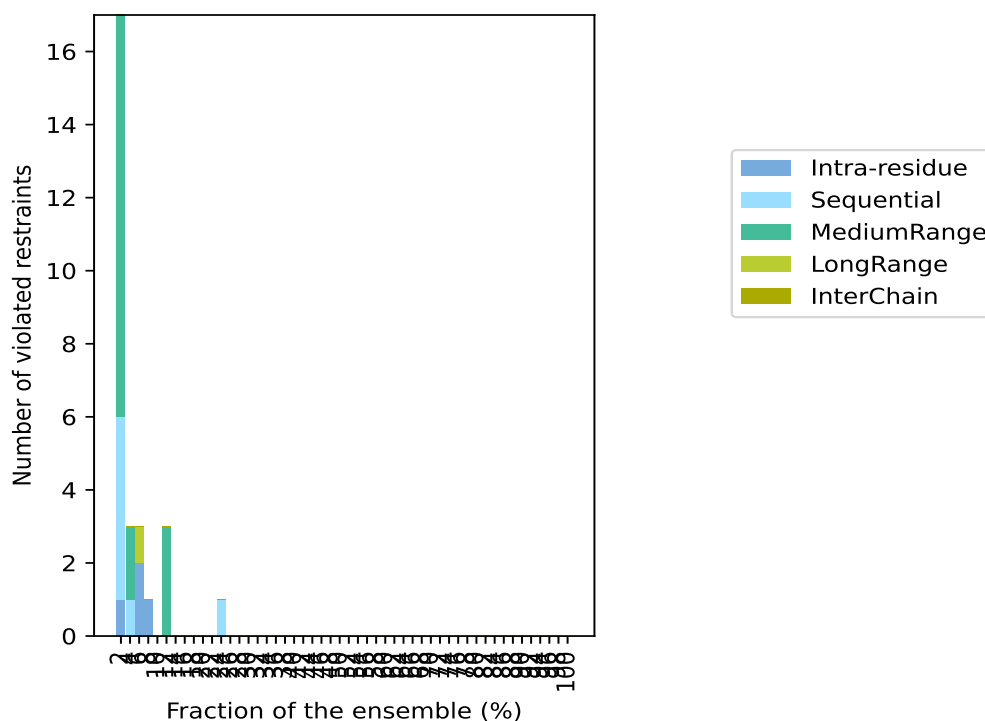
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	48	96.0
0	0	0	0	0	0	49	98.0
0	0	0	0	0	0	50	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

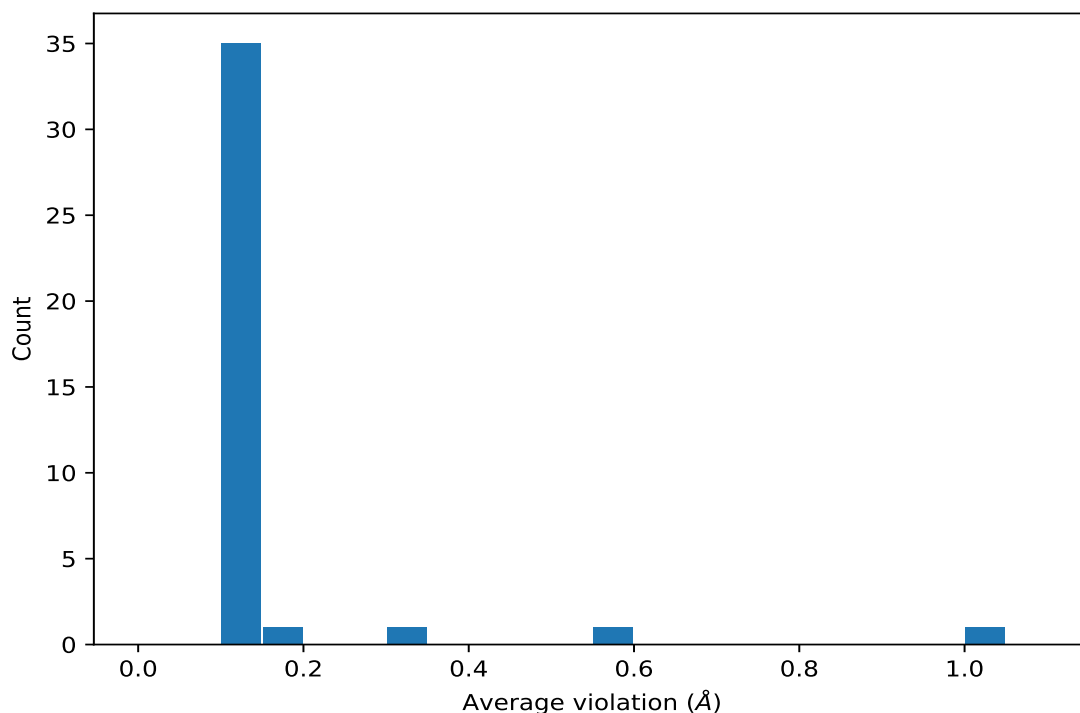
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	44	1.01	0.27	1.12
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	41	0.6	0.16	0.62
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	18	0.34	0.1	0.34
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	12	0.15	0.02	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	12	0.15	0.02	0.14
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	8	0.16	0.05	0.16
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	6	0.13	0.02	0.14
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	6	0.13	0.02	0.14
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	6	0.12	0.0	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	6	0.12	0.0	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	6	0.12	0.0	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	6	0.12	0.0	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	6	0.12	0.0	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	6	0.12	0.0	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	6	0.12	0.0	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	6	0.12	0.0	0.12

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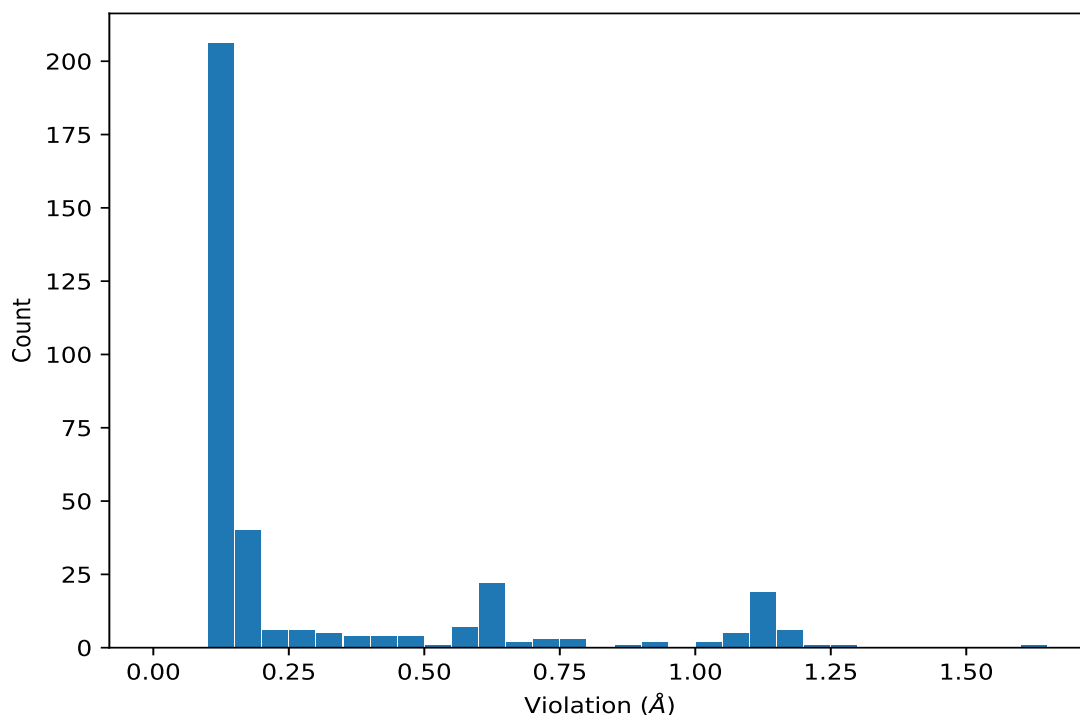
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	6	0.12	0.0	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	6	0.12	0.0	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	6	0.12	0.0	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	6	0.12	0.0	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD1	4	0.14	0.03	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD2	4	0.14	0.03	0.12
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE1	3	0.13	0.02	0.12
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE2	3	0.13	0.02	0.12
(1,405)	1:A:23:PHE:HE1	1:A:23:PHE:H	3	0.13	0.02	0.12
(1,405)	1:A:23:PHE:HE2	1:A:23:PHE:H	3	0.13	0.02	0.12
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD2	3	0.13	0.0	0.13
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD3	3	0.13	0.0	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD2	3	0.13	0.0	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD3	3	0.13	0.0	0.13
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ1	2	0.15	0.04	0.15
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ2	2	0.15	0.04	0.15
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ3	2	0.15	0.04	0.15
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD1	2	0.14	0.02	0.14
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD2	2	0.14	0.02	0.14
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD1	2	0.14	0.02	0.14
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD2	2	0.14	0.02	0.14
(1,1623)	1:A:23:PHE:HA	1:A:19:LEU:HA	2	0.12	0.01	0.12
(2,17)	1:A:22:GLY:O	1:A:26:PHE:H	2	0.12	0.01	0.12

<sup>1</sup>Number of violated models, <sup>2</sup>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 lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	50	1.62
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	35	1.25
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	41	1.22
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	44	1.19
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	50	1.17
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	48	1.17
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	36	1.16
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	3	1.15
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	42	1.15
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	11	1.14
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	20	1.14
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	4	1.13
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	23	1.13
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	26	1.13
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	37	1.13
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	38	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	1	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	2	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	9	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	10	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	13	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	27	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	28	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	46	1.12
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	6	1.11
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	15	1.1
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	32	1.1
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	33	1.1
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	24	1.09
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	34	1.08
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	21	1.07
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	22	1.06
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	25	1.06
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	40	1.04
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	49	1.02
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	39	0.93
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	5	0.9
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	47	0.89
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	35	0.78
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	41	0.76
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	44	0.75
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	42	0.72
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	48	0.72
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	28	0.7
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	32	0.67
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	36	0.65
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	3	0.64
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	11	0.64
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	20	0.64
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	4	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	6	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	9	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	23	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	24	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	37	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	38	0.63
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	1	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	10	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	13	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	15	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	26	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	27	0.62
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	25	0.61
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	34	0.61
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	8	0.61
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	14	0.61
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	46	0.6
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	21	0.59
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	22	0.59
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	33	0.59
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	40	0.58
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	46	0.57
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	47	0.55
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	49	0.55
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	7	0.5
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	39	0.49
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	5	0.48
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	45	0.45
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	30	0.45
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	19	0.43
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	29	0.43
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	31	0.43
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	39	0.43
(2,9)	1:A:17:THR:O	1:A:21:PHE:H	26	0.39
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	42	0.38
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	48	0.38
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	43	0.35
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	12	0.34
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	50	0.34
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	35	0.33
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	41	0.33
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	8	0.3
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	8	0.29
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	14	0.29
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	46	0.29
(2,19)	1:A:23:PHE:O	1:A:27:LYS:H	17	0.26
(1,1080)	1:A:27:LYS:H	1:A:26:PHE:HD1	46	0.26
(1,1080)	1:A:27:LYS:H	1:A:26:PHE:HD2	46	0.26
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	7	0.23
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	14	0.22
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	12	0.21
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	7	0.2
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	17	0.2
(2,13)	1:A:19:LEU:O	1:A:23:PHE:H	28	0.19
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD1	33	0.19
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD2	33	0.19
(1,1530)	1:A:29:LEU:H	1:A:32:LYS:HB2	34	0.19
(1,1530)	1:A:29:LEU:H	1:A:32:LYS:HB3	34	0.19
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	28	0.19
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	28	0.19
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	50	0.19
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	50	0.19
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ1	49	0.19
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ2	49	0.19
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ3	49	0.19
(2,20)	1:A:23:PHE:O	1:A:27:LYS:N	45	0.18
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	30	0.17
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	44	0.17
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	44	0.17
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	32	0.17
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	32	0.17
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	29	0.16
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	31	0.16
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	39	0.16
(2,10)	1:A:17:THR:O	1:A:21:PHE:N	26	0.16
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	31	0.16
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	31	0.16
(2,7)	1:A:14:ALA:O	1:A:18:PHE:H	26	0.15
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	19	0.15
(1,405)	1:A:23:PHE:HE1	1:A:23:PHE:H	50	0.15
(1,405)	1:A:23:PHE:HE2	1:A:23:PHE:H	50	0.15
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE1	50	0.15
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE2	50	0.15
(1,1529)	1:A:29:LEU:HA	1:A:32:LYS:HG2	24	0.15
(1,1529)	1:A:29:LEU:HA	1:A:32:LYS:HG3	24	0.15
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD1	43	0.15
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD2	43	0.15
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD1	43	0.15
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD2	43	0.15
(1,1282)	1:A:30:GLN:HB2	1:A:32:LYS:HE2	33	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:A:30:GLN:HB2	1:A:32:LYS:HE3	33	0.15
(1,1282)	1:A:30:GLN:HB3	1:A:32:LYS:HE2	33	0.15
(1,1282)	1:A:30:GLN:HB3	1:A:32:LYS:HE3	33	0.15
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	26	0.14
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	26	0.14
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	31	0.14
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	31	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	10	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	10	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	11	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	11	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	13	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	13	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	20	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	20	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	44	0.14
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	44	0.14
(2,17)	1:A:22:GLY:O	1:A:26:PHE:H	35	0.13
(1,395)	1:A:23:PHE:H	1:A:23:PHE:HD1	50	0.13
(1,395)	1:A:23:PHE:H	1:A:23:PHE:HD2	50	0.13
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD2	35	0.13
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD3	35	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD2	35	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD3	35	0.13
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD2	48	0.13
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD3	48	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD2	48	0.13
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD3	48	0.13
(1,1623)	1:A:23:PHE:HA	1:A:19:LEU:HA	28	0.13
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	48	0.13
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	48	0.13
(1,1179)	1:A:5:ILE:H	1:A:3:HIS:HE1	27	0.13
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	26	0.13
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	26	0.13
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	27	0.13
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	27	0.13
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	42	0.12
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD11	40	0.12
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD12	40	0.12
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD13	40	0.12
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD21	40	0.12
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD22	40	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:A:18:PHE:HE1	1:A:19:LEU:HD23	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD11	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD12	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD13	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD21	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD22	40	0.12
(1,959)	1:A:18:PHE:HE2	1:A:19:LEU:HD23	40	0.12
(1,955)	1:A:19:LEU:HD11	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD11	1:A:18:PHE:HE2	40	0.12
(1,955)	1:A:19:LEU:HD12	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD12	1:A:18:PHE:HE2	40	0.12
(1,955)	1:A:19:LEU:HD13	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD13	1:A:18:PHE:HE2	40	0.12
(1,955)	1:A:19:LEU:HD21	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD21	1:A:18:PHE:HE2	40	0.12
(1,955)	1:A:19:LEU:HD22	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD22	1:A:18:PHE:HE2	40	0.12
(1,955)	1:A:19:LEU:HD23	1:A:18:PHE:HE1	40	0.12
(1,955)	1:A:19:LEU:HD23	1:A:18:PHE:HE2	40	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD1	17	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD2	17	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD1	34	0.12
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD2	34	0.12
(1,405)	1:A:23:PHE:HE1	1:A:23:PHE:H	46	0.12
(1,405)	1:A:23:PHE:HE2	1:A:23:PHE:H	46	0.12
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE1	46	0.12
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE2	46	0.12
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD2	41	0.12
(1,1701)	1:A:22:GLY:HA2	1:A:27:LYS:HD3	41	0.12
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD2	41	0.12
(1,1701)	1:A:22:GLY:HA3	1:A:27:LYS:HD3	41	0.12
(1,1623)	1:A:23:PHE:HA	1:A:19:LEU:HA	40	0.12
(1,1622)	1:A:21:PHE:HA	1:A:17:THR:HA	49	0.12
(1,1605)	1:A:18:PHE:HA	1:A:14:ALA:HB1	26	0.12
(1,1605)	1:A:18:PHE:HA	1:A:14:ALA:HB2	26	0.12
(1,1605)	1:A:18:PHE:HA	1:A:14:ALA:HB3	26	0.12
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD1	47	0.12
(1,1504)	1:A:29:LEU:HB2	1:A:26:PHE:HD2	47	0.12
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD1	47	0.12
(1,1504)	1:A:29:LEU:HB3	1:A:26:PHE:HD2	47	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	6	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	6	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	6	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	6	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	6	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	20	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	20	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	20	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	20	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	20	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	20	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	47	0.12
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	47	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	47	0.12
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	47	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	47	0.12
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	47	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	6	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	6	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	6	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	6	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	6	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	6	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	20	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	20	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	20	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	20	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	20	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	20	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	47	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	47	0.12
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	47	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	47	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	47	0.12
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	47	0.12
(1,1286)	1:A:7:GLU:HB2	1:A:4:THR:H	37	0.12
(1,1286)	1:A:7:GLU:HB3	1:A:4:THR:H	37	0.12
(1,1264)	1:A:28:TYR:HD1	1:A:30:GLN:H	40	0.12
(1,1264)	1:A:28:TYR:HD2	1:A:30:GLN:H	40	0.12
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD1	34	0.12
(1,1135)	1:A:29:LEU:HG	1:A:28:TYR:HD2	34	0.12
(1,1085)	1:A:26:PHE:HD1	1:A:27:LYS:HG2	18	0.12
(1,1085)	1:A:26:PHE:HD1	1:A:27:LYS:HG3	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:A:26:PHE:HD2	1:A:27:LYS:HG2	18	0.12
(1,1085)	1:A:26:PHE:HD2	1:A:27:LYS:HG3	18	0.12
(1,1079)	1:A:27:LYS:HG2	1:A:26:PHE:HD1	18	0.12
(1,1079)	1:A:27:LYS:HG2	1:A:26:PHE:HD2	18	0.12
(1,1079)	1:A:27:LYS:HG3	1:A:26:PHE:HD1	18	0.12
(1,1079)	1:A:27:LYS:HG3	1:A:26:PHE:HD2	18	0.12
(2,17)	1:A:22:GLY:O	1:A:26:PHE:H	41	0.11
(2,14)	1:A:19:LEU:O	1:A:23:PHE:N	48	0.11
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD1	43	0.11
(1,575)	1:A:28:TYR:HA	1:A:28:TYR:HD2	43	0.11
(1,405)	1:A:23:PHE:HE1	1:A:23:PHE:H	39	0.11
(1,405)	1:A:23:PHE:HE2	1:A:23:PHE:H	39	0.11
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE1	39	0.11
(1,404)	1:A:23:PHE:H	1:A:23:PHE:HE2	39	0.11
(1,1711)	1:A:25:LEU:HD11	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD11	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:25:LEU:HD12	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD12	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:25:LEU:HD13	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD13	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:25:LEU:HD21	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD21	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:25:LEU:HD22	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD22	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:25:LEU:HD23	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:25:LEU:HD23	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD11	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD11	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD12	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD12	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD13	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD13	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD21	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD21	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD22	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD22	1:A:28:TYR:HE2	47	0.11
(1,1711)	1:A:29:LEU:HD23	1:A:28:TYR:HE1	47	0.11
(1,1711)	1:A:29:LEU:HD23	1:A:28:TYR:HE2	47	0.11
(1,1674)	1:A:29:LEU:H	1:A:25:LEU:HG	49	0.11
(1,1672)	1:A:25:LEU:HG	1:A:29:LEU:H	49	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	9	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	9	0.11
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	9	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	9	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	9	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	21	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	21	0.11
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	21	0.11
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	21	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	21	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	21	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB2	44	0.11
(1,1353)	1:A:10:ALA:HB1	1:A:7:GLU:HB3	44	0.11
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB2	44	0.11
(1,1353)	1:A:10:ALA:HB2	1:A:7:GLU:HB3	44	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB2	44	0.11
(1,1353)	1:A:10:ALA:HB3	1:A:7:GLU:HB3	44	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	9	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	9	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	9	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	9	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	9	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	9	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	21	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	21	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	21	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	21	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	21	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	21	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB1	44	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB2	44	0.11
(1,1352)	1:A:7:GLU:HB2	1:A:10:ALA:HB3	44	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB1	44	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB2	44	0.11
(1,1352)	1:A:7:GLU:HB3	1:A:10:ALA:HB3	44	0.11
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	30	0.11
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	30	0.11
(1,1273)	1:A:31:LYS:HD2	1:A:29:LEU:HA	42	0.11
(1,1273)	1:A:31:LYS:HD3	1:A:29:LEU:HA	42	0.11
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ1	47	0.11
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ2	47	0.11
(1,1126)	1:A:28:TYR:H	1:A:27:LYS:HZ3	47	0.11

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

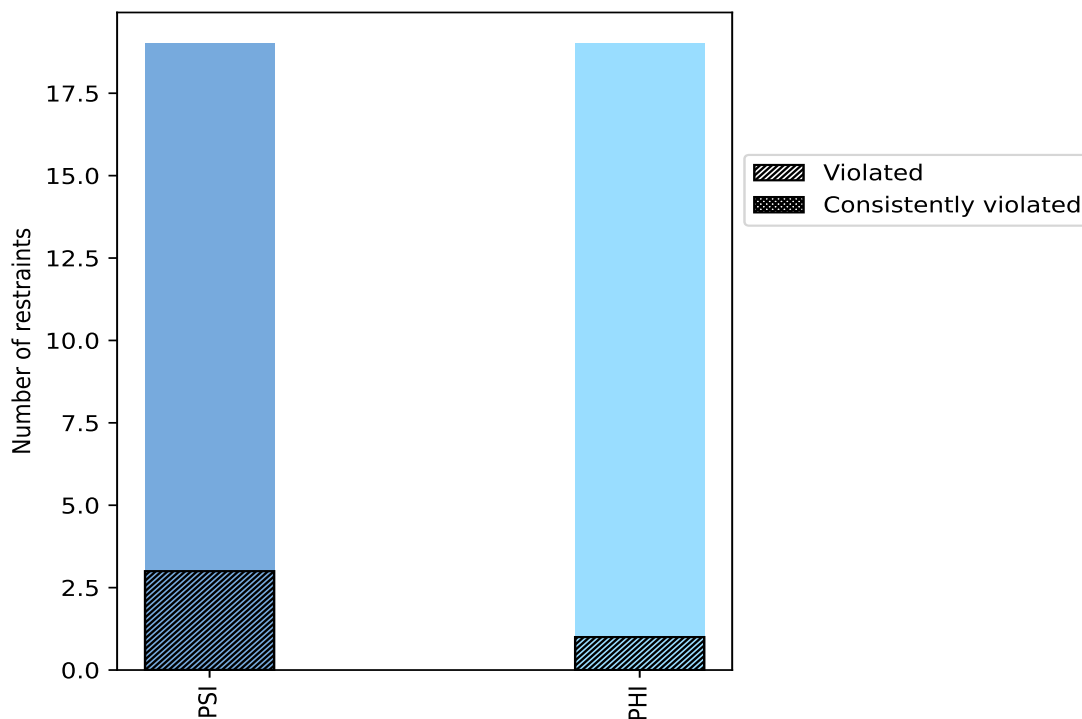
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	19	50.0	3	15.8	7.9	0	0.0	0.0
PHI	19	50.0	1	5.3	2.6	0	0.0	0.0
Total	38	100.0	4	10.5	10.5	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 [\(i\)](#)

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

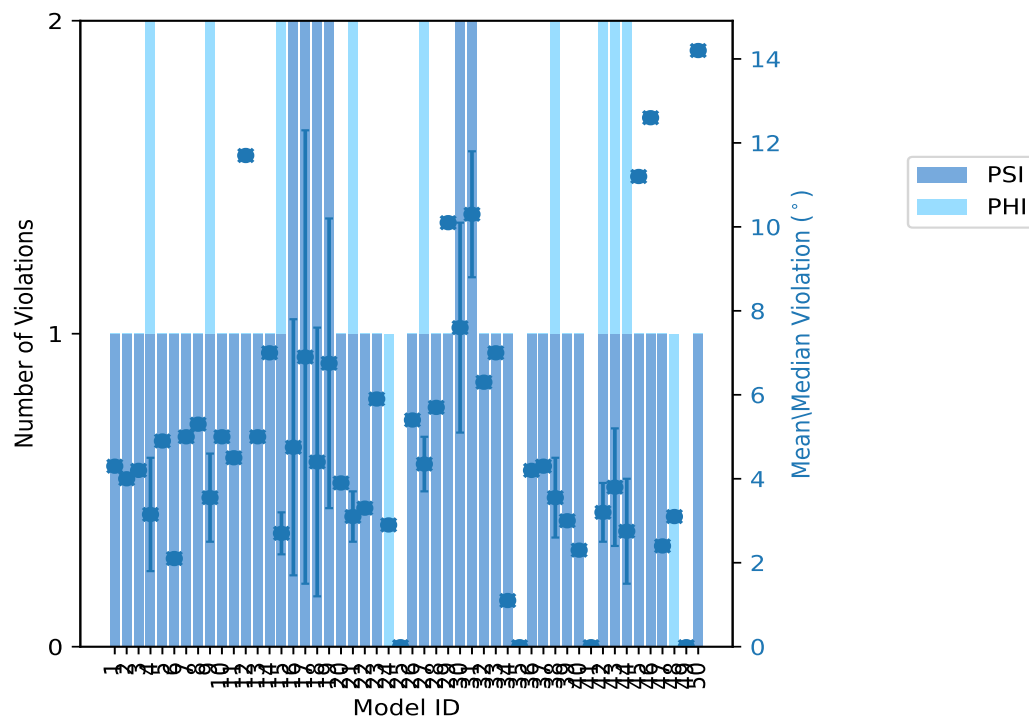
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	0	1	4.3	4.3	0.0	4.3
2	1	0	1	4.0	4.0	0.0	4.0
3	1	0	1	4.2	4.2	0.0	4.2
4	1	1	2	3.15	4.5	1.35	3.15
5	1	0	1	4.9	4.9	0.0	4.9
6	1	0	1	2.1	2.1	0.0	2.1
7	1	0	1	5.0	5.0	0.0	5.0
8	1	0	1	5.3	5.3	0.0	5.3
9	1	1	2	3.55	4.6	1.05	3.55
10	1	0	1	5.0	5.0	0.0	5.0
11	1	0	1	4.5	4.5	0.0	4.5
12	1	0	1	11.7	11.7	0.0	11.7
13	1	0	1	5.0	5.0	0.0	5.0
14	1	0	1	7.0	7.0	0.0	7.0
15	1	1	2	2.7	3.2	0.5	2.7
16	2	0	2	4.75	7.8	3.05	4.75
17	2	0	2	6.9	12.3	5.4	6.9
18	2	0	2	4.4	7.6	3.2	4.4
19	2	0	2	6.75	10.2	3.45	6.75
20	1	0	1	3.9	3.9	0.0	3.9
21	1	1	2	3.1	3.7	0.6	3.1
22	1	0	1	3.3	3.3	0.0	3.3
23	1	0	1	5.9	5.9	0.0	5.9
24	0	1	1	2.9	2.9	0.0	2.9
25	0	0	0	0.0	0.0	0.0	0.0
26	1	0	1	5.4	5.4	0.0	5.4
27	1	1	2	4.35	5.0	0.65	4.35
28	1	0	1	5.7	5.7	0.0	5.7
29	1	0	1	10.1	10.1	0.0	10.1
30	2	0	2	7.6	10.1	2.5	7.6
31	2	0	2	10.3	11.8	1.5	10.3
32	1	0	1	6.3	6.3	0.0	6.3
33	1	0	1	7.0	7.0	0.0	7.0
34	1	0	1	1.1	1.1	0.0	1.1
35	0	0	0	0.0	0.0	0.0	0.0
36	1	0	1	4.2	4.2	0.0	4.2
37	1	0	1	4.3	4.3	0.0	4.3
38	1	1	2	3.55	4.5	0.95	3.55

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	1	0	1	3.0	3.0	0.0	3.0
40	1	0	1	2.3	2.3	0.0	2.3
41	0	0	0	0.0	0.0	0.0	0.0
42	1	1	2	3.2	3.9	0.7	3.2
43	1	1	2	3.8	5.2	1.4	3.8
44	1	1	2	2.75	4.0	1.25	2.75
45	1	0	1	11.2	11.2	0.0	11.2
46	1	0	1	12.6	12.6	0.0	12.6
47	1	0	1	2.4	2.4	0.0	2.4
48	0	1	1	3.1	3.1	0.0	3.1
49	0	0	0	0.0	0.0	0.0	0.0
50	1	0	1	14.2	14.2	0.0	14.2

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

### 10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	1	2.0
0	0	0	2	4.0
0	0	0	3	6.0
0	0	0	4	8.0
0	0	0	5	10.0
1	0	1	6	12.0
0	0	0	7	14.0
0	0	0	8	16.0
0	0	0	9	18.0
1	0	1	10	20.0
0	1	1	11	22.0
0	0	0	12	24.0
0	0	0	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	0	0	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
0	0	0	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
1	0	1	34	68.0
0	0	0	35	70.0
0	0	0	36	72.0
0	0	0	37	74.0

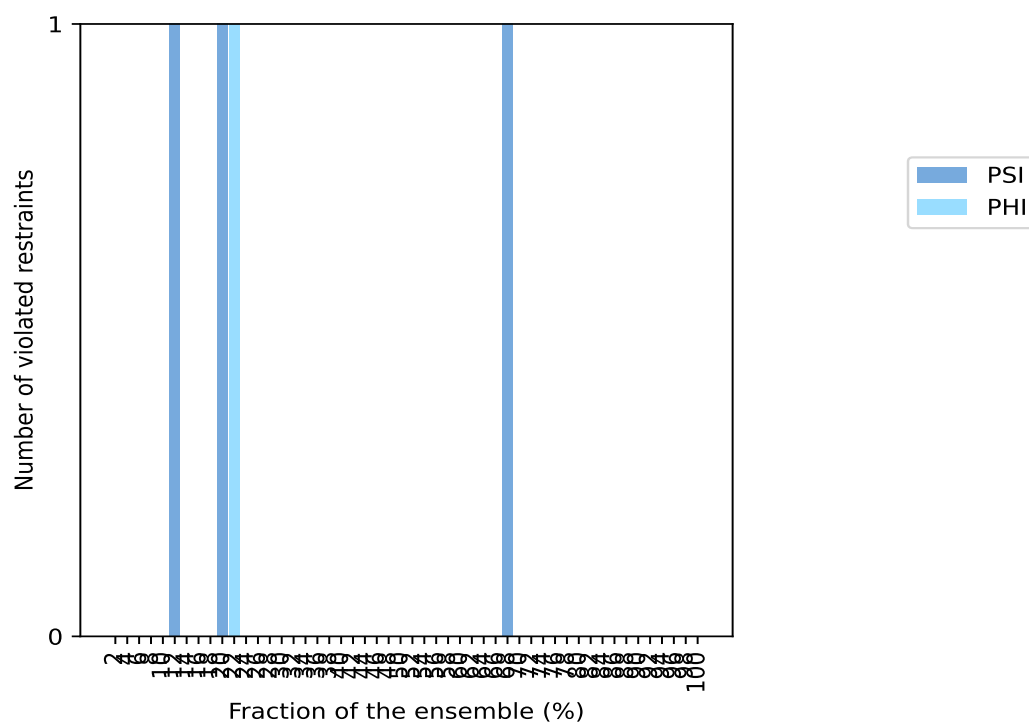
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

<sup>1</sup> Number of models with violations

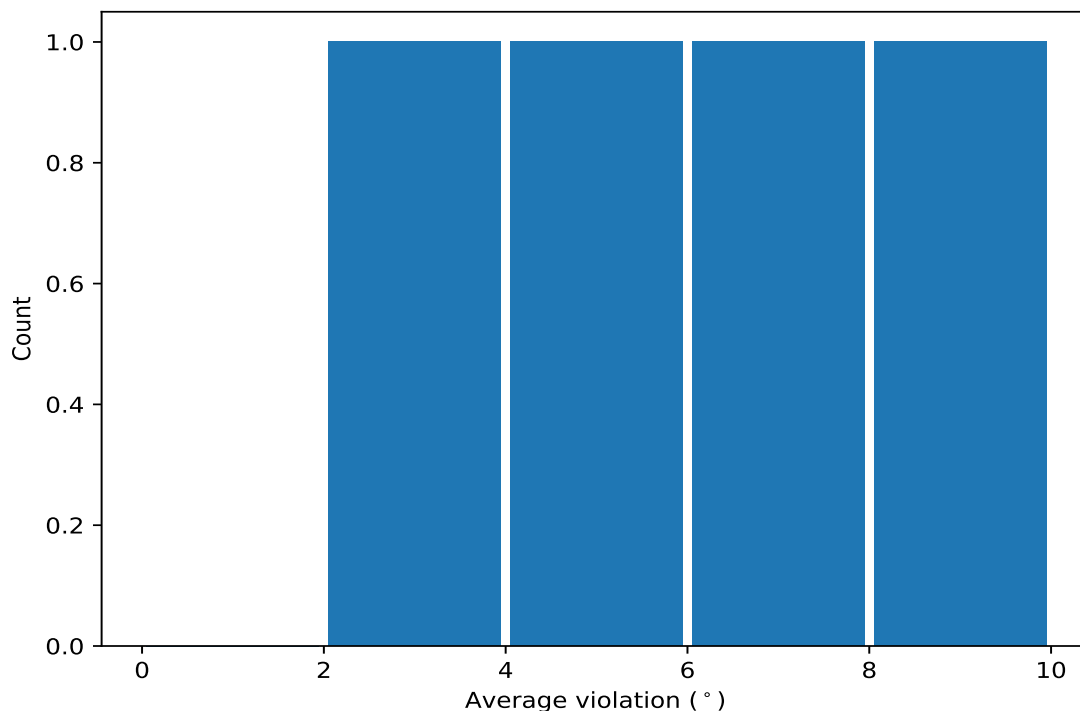
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	34	4.6	2.16	4.5
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	11	2.52	0.57	2.5
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	10	7.48	4.57	8.15
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	6	9.1	1.1	9.45

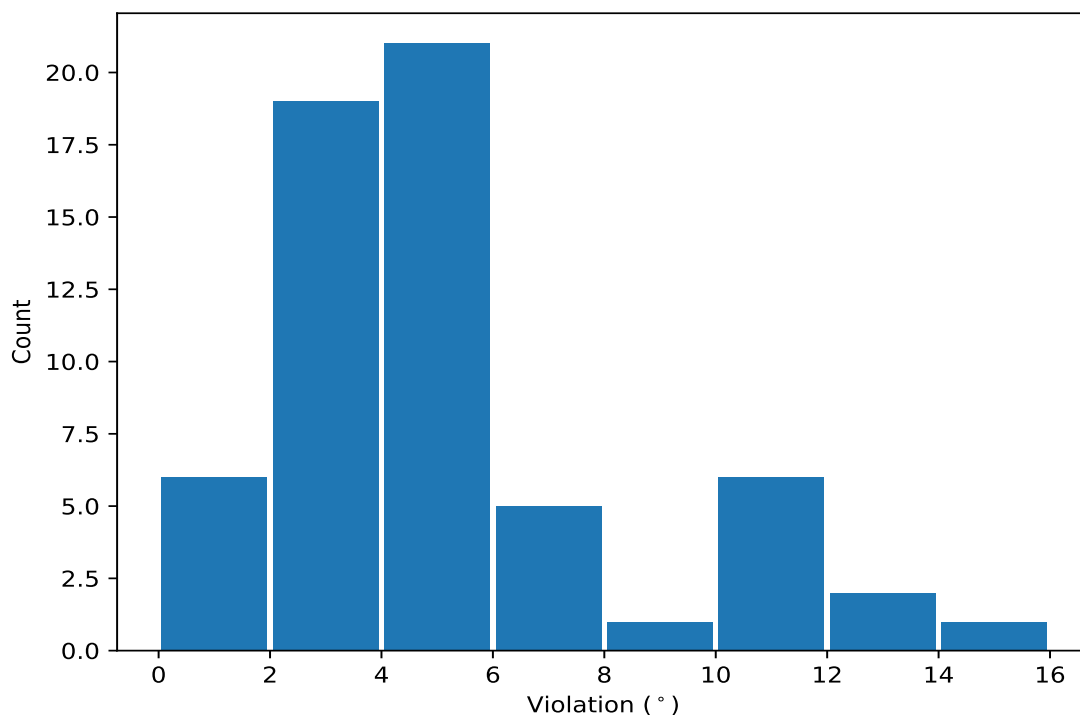
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)



## 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 lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	50	14.2
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	46	12.6
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	17	12.3
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	31	11.8
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	12	11.7
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	45	11.2
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	19	10.2
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	29	10.1
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	30	10.1
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	31	8.8
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	16	7.8
(1,30)	1:A:23:PHE:N	1:A:23:PHE:CA	1:A:23:PHE:C	1:A:24:TRP:N	18	7.6
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	14	7.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	33	7.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	32	6.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	23	5.9
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	28	5.7
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	26	5.4
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	8	5.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	43	5.2
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	30	5.1
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	7	5.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	10	5.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	13	5.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	27	5.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	5	4.9
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	9	4.6
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	4	4.5
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	11	4.5
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	38	4.5
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	1	4.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	37	4.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	3	4.2
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	36	4.2
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	2	4.0
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	44	4.0
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	42	3.9
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	20	3.9
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	21	3.7
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	27	3.7
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	19	3.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	22	3.3
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	15	3.2
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	48	3.1
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	39	3.0
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	24	2.9
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	38	2.6
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	9	2.5
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	21	2.5
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	42	2.5
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	47	2.4
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	43	2.4
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	40	2.3
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	15	2.2
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	6	2.1
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	4	1.8
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	16	1.7
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	17	1.5
(1,17)	1:A:16:LEU:C	1:A:17:THR:N	1:A:17:THR:CA	1:A:17:THR:C	44	1.5
(1,38)	1:A:27:LYS:N	1:A:27:LYS:CA	1:A:27:LYS:C	1:A:28:TYR:N	18	1.2
(1,36)	1:A:26:PHE:N	1:A:26:PHE:CA	1:A:26:PHE:C	1:A:27:LYS:N	34	1.1