WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 12:24 PM EST

PDB ID	:	2JY9
BMRB ID	:	15584
Title	:	NMR structure of putative tRNA hydrolase domain from Salmonella typhimurium. NorthEast Structural Genomics Consortium target StR220
Authors	:	Singarapu, K.K.; Wu, Y.; Sukumaran, D.; Eletsky, A.; Zeri, A.; Wang, D.; Janjua, H.; Owens, L.; Xiao, R.; Liu, J.; Baran, M.C.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-12-07

The following versions of software and data (see references ⓘ) were used in the production of this report:
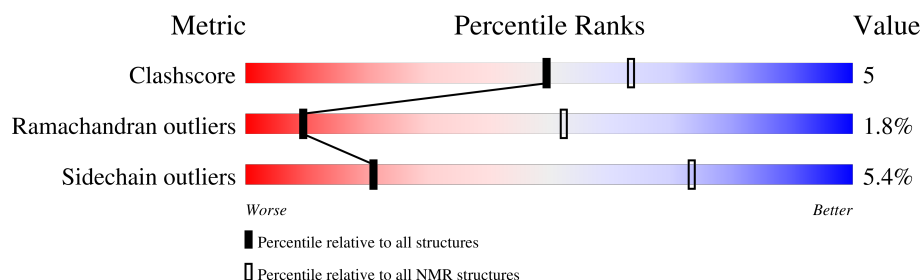
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 87%.

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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		1.8%
Sidechain outliers		5.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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

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

Mol	Chain	Length	Quality of chain
1	A	148	66% 5% 28%

2 Ensemble composition and analysis ⓘ

This entry contains 20 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: *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:1-A:21, A:36-A:100 (86)	1.15	10
2	A:126-A:145 (20)	2.04	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 2 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2403 atoms, of which 1229 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative tRNA hydrolase domain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2403	722	1229	239	212	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	-	expression tag	UNP Q8ZRN3
A	142	GLU	-	expression tag	UNP Q8ZRN3
A	143	HIS	-	expression tag	UNP Q8ZRN3
A	144	HIS	-	expression tag	UNP Q8ZRN3
A	145	HIS	-	expression tag	UNP Q8ZRN3
A	146	HIS	-	expression tag	UNP Q8ZRN3
A	147	HIS	-	expression tag	UNP Q8ZRN3
A	148	HIS	-	expression tag	UNP Q8ZRN3

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.
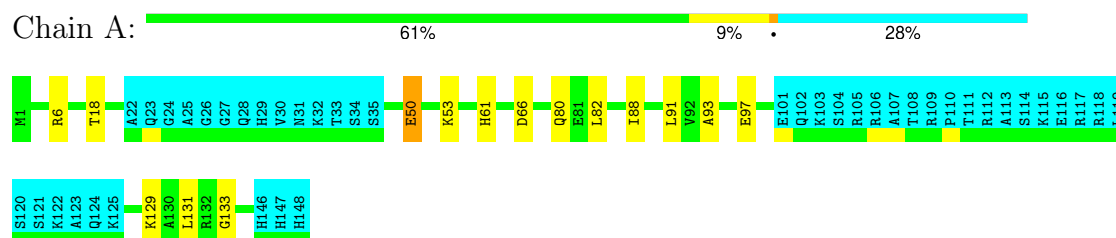
• Molecule 1: Putative tRNA hydrolase domain
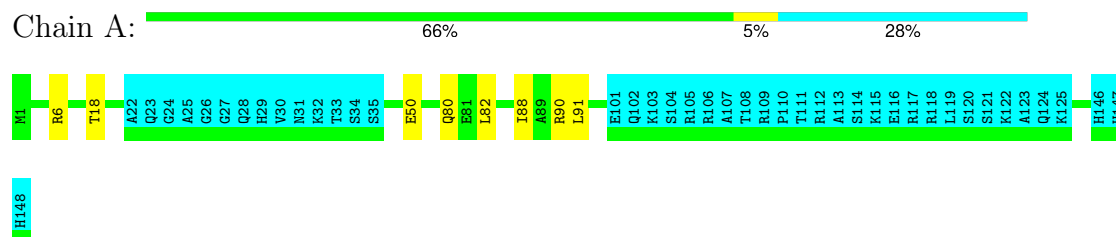
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Putative tRNA hydrolase domain

4.2.2 Score per residue for model 2

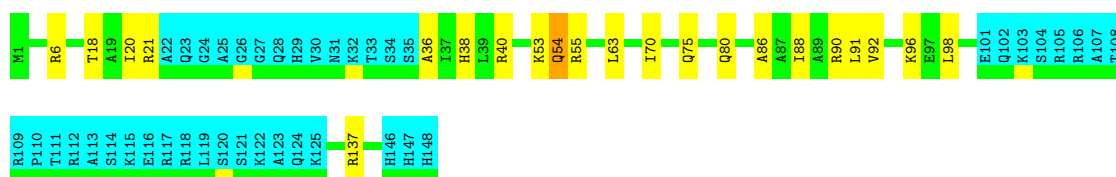• Molecule 1: Putative tRNA hydrolase domain

4.2.3 Score per residue for model 3

• Molecule 1: Putative tRNA hydrolase domain

4.2.4 Score per residue for model 4

• Molecule 1: Putative tRNA hydrolase domain

4.2.5 Score per residue for model 5

• Molecule 1: Putative tRNA hydrolase domain

4.2.6 Score per residue for model 6

• Molecule 1: Putative tRNA hydrolase domain

Chain A: 55%   16% • 28%

4.2.7 Score per residue for model 7

● Molecule 1: Putative tRNA hydrolase domain

Chain A: 55%   15% • 28%

4.2.8 Score per residue for model 8

● Molecule 1: Putative tRNA hydrolase domain

Chain A: 59%   12%   28%

4.2.9 Score per residue for model 9

● Molecule 1: Putative tRNA hydrolase domain

Chain A: 60%   11% • 28%

4.2.10   Score per residue for model 10 (medoid)

• Molecule 1: Putative tRNA hydrolase domain

Chain A:

4.2.11   Score per residue for model 11

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
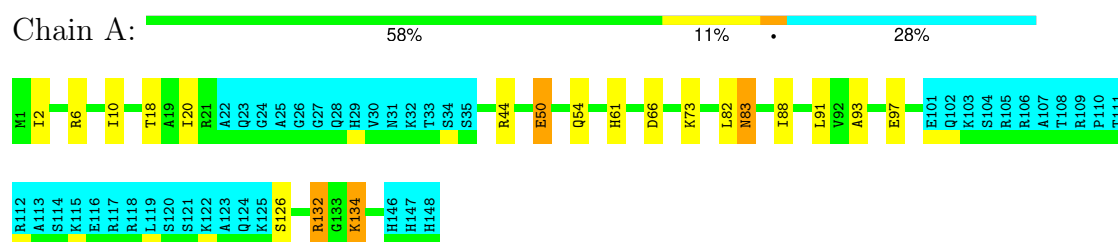
4.2.12   Score per residue for model 12
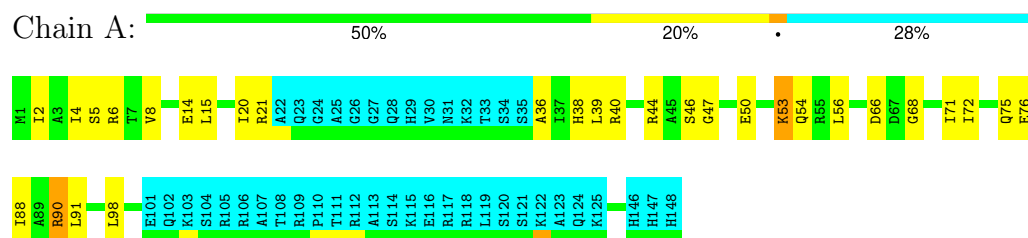
• Molecule 1: Putative tRNA hydrolase domain
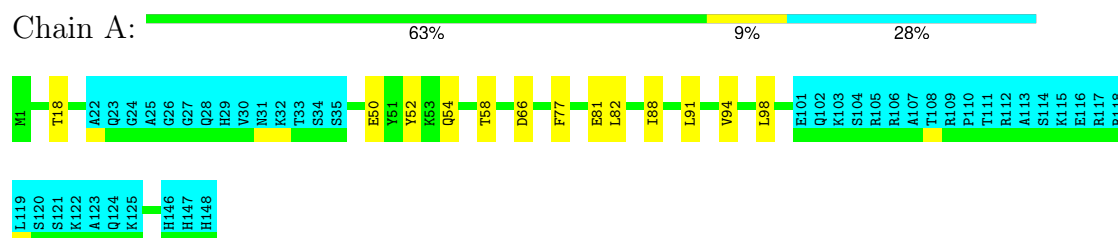
Chain A:
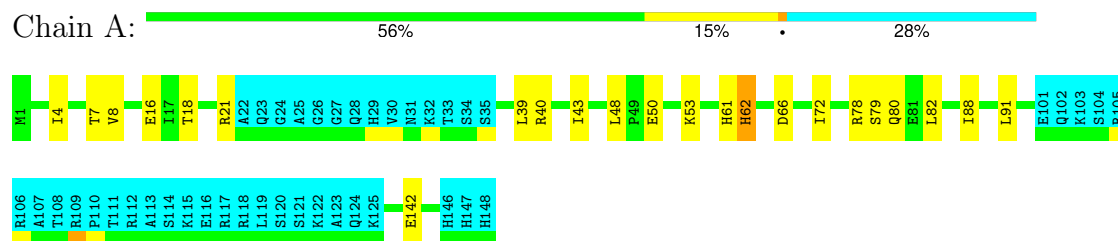
4.2.13   Score per residue for model 13

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
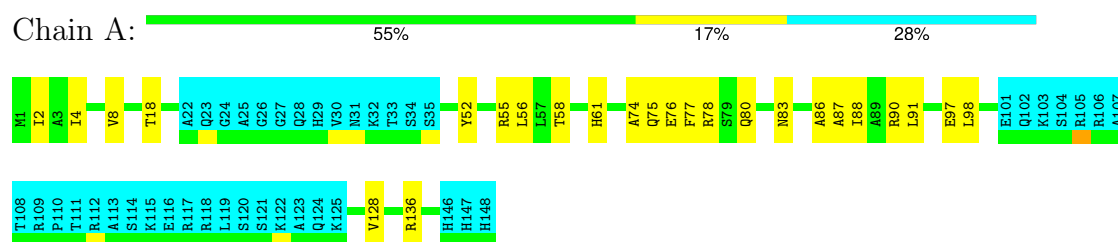
4.2.14 Score per residue for model 14

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
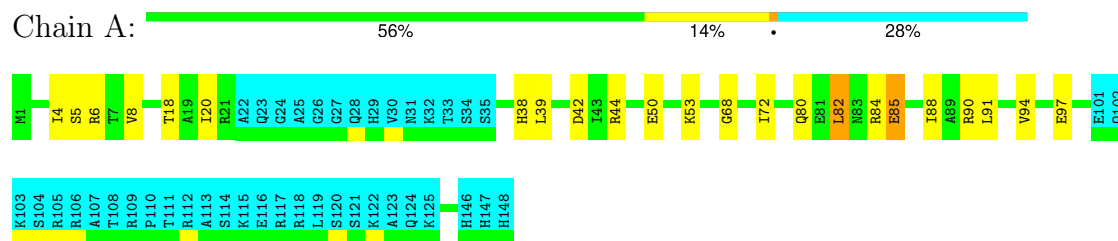
4.2.15 Score per residue for model 15

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
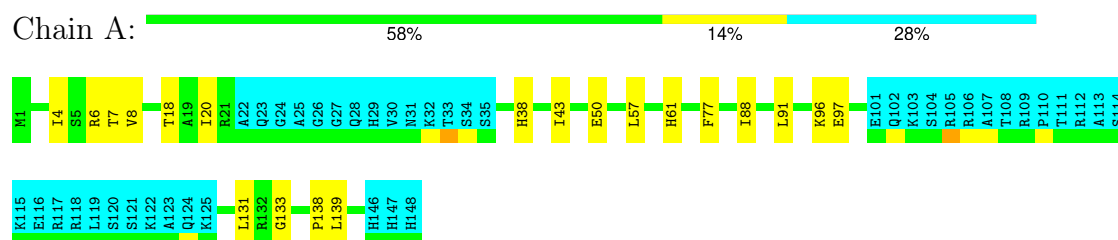
4.2.16 Score per residue for model 16

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
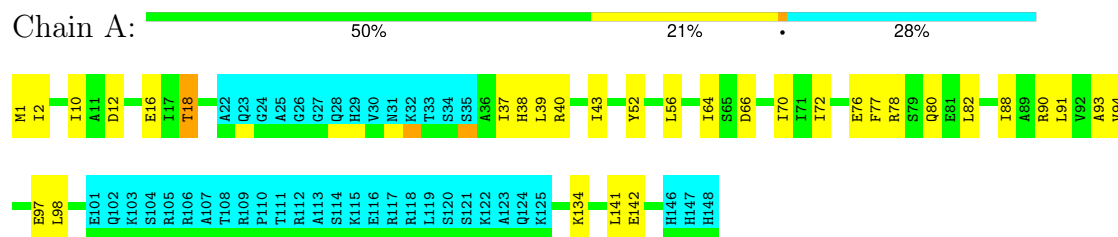
4.2.17 Score per residue for model 17

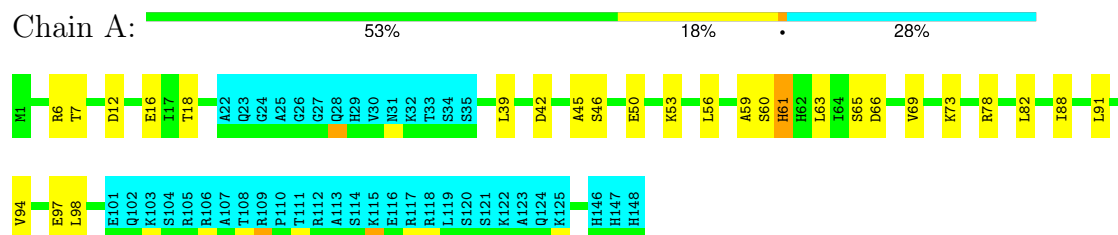• Molecule 1: Putative tRNA hydrolase domain

Chain A:
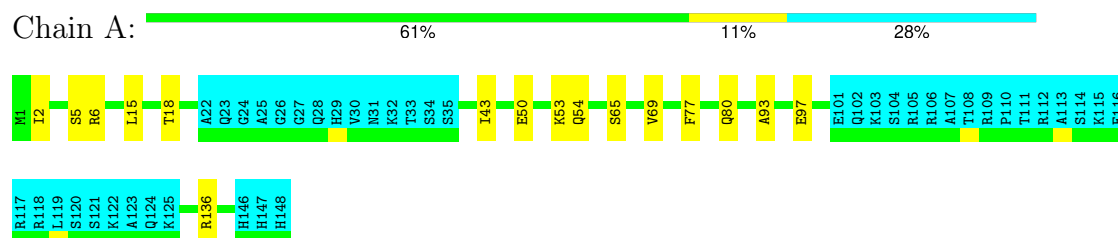
4.2.18   Score per residue for model 18

• Molecule 1: Putative tRNA hydrolase domain

Chain A:
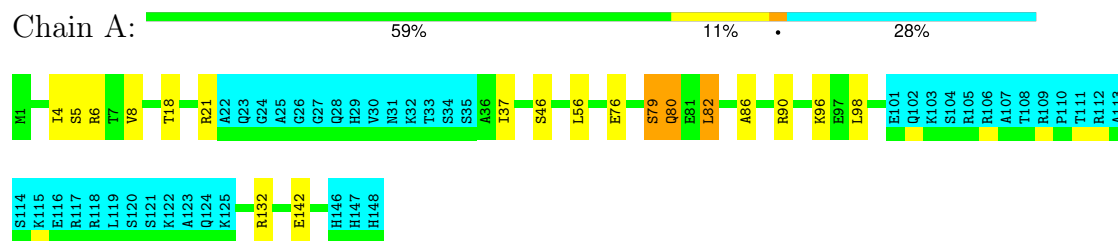
4.2.19   Score per residue for model 19

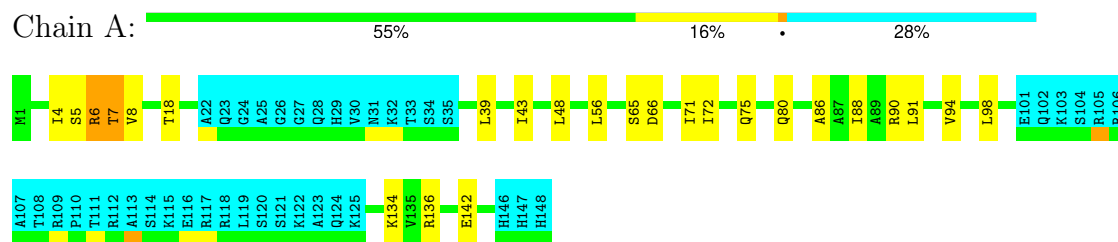• Molecule 1: Putative tRNA hydrolase domain

Chain A:
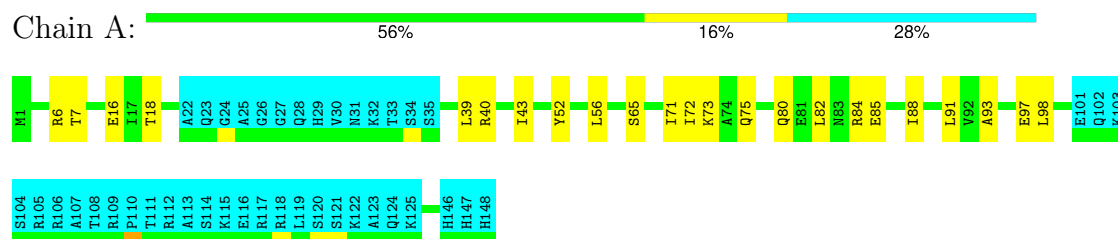
4.2.20   Score per residue for model 20

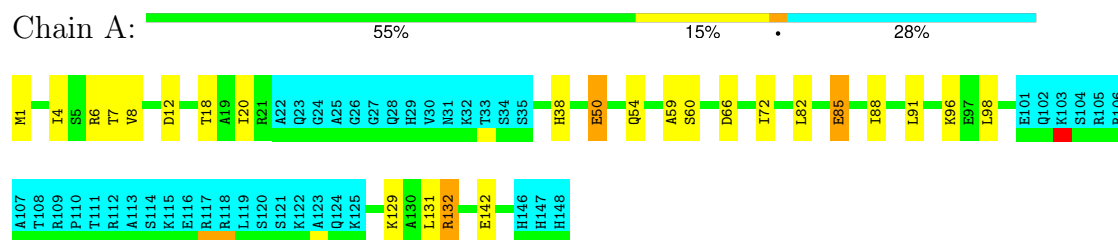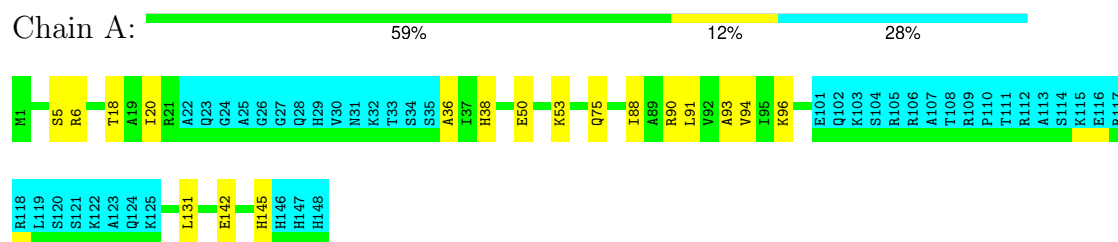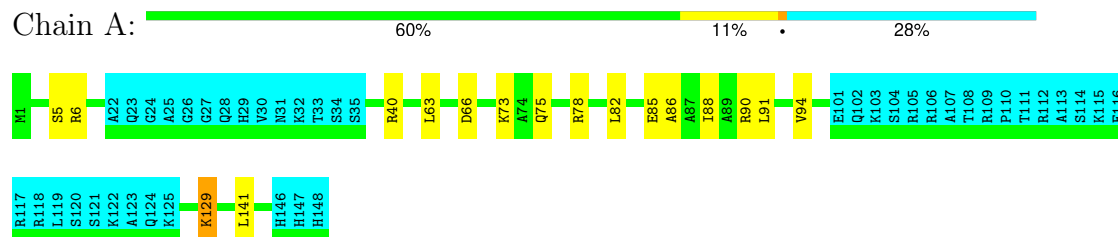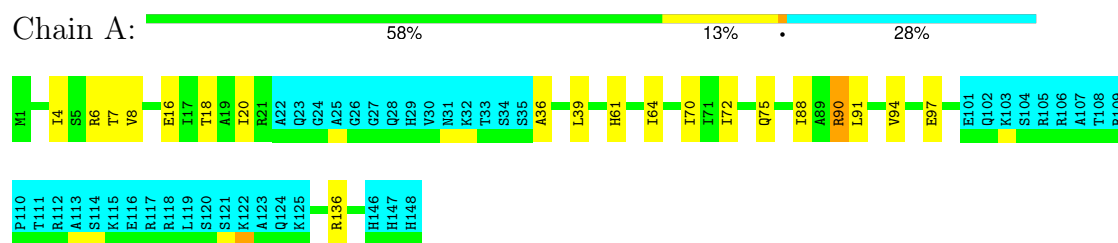• Molecule 1: Putative tRNA hydrolase domain

Chain A:
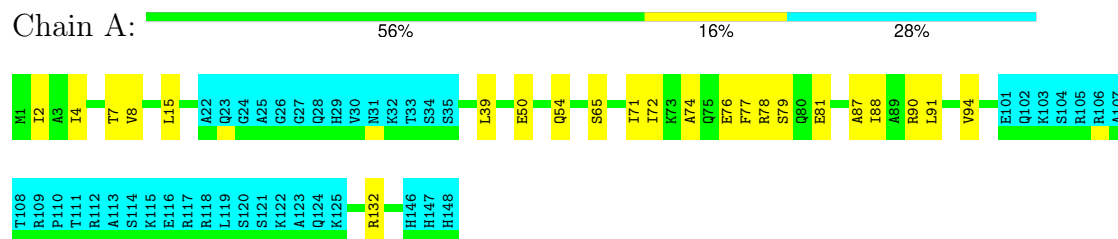
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
CYANA	refinement	
MOLMOL	structure solution	

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	1702
Number of shifts mapped to atoms	1702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	844	892	886	10±3
All	All	16880	17840	17720	190

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:65:SER:HB3	1:A:69:VAL:HG13	0.86	1.45	5	2
1:A:50:GLU:HA	1:A:53:LYS:HE2	0.83	1.48	1	2
1:A:59:ALA:HA	1:A:98:LEU:HG	0.77	1.55	7	1
1:A:16:GLU:HB2	1:A:40:ARG:HB3	0.70	1.63	19	2
1:A:82:LEU:HA	1:A:85:GLU:HG2	0.68	1.65	9	4
1:A:50:GLU:HG3	1:A:53:LYS:HD2	0.68	1.64	3	1
1:A:129:LYS:HE3	1:A:129:LYS:HA	0.68	1.65	9	1
1:A:2:ILE:HD11	1:A:15:LEU:HD11	0.67	1.67	3	3
1:A:42:ASP:HB3	1:A:69:VAL:HB	0.67	1.65	5	1
1:A:4:ILE:HB	1:A:8:VAL:HG13	0.66	1.68	20	3
1:A:54:GLN:HA	1:A:54:GLN:HE21	0.65	1.51	2	1
1:A:78:ARG:HG2	1:A:79:SER:H	0.62	1.54	12	2
1:A:43:ILE:HG12	1:A:56:LEU:HD13	0.61	1.71	19	1
1:A:56:LEU:HD23	1:A:98:LEU:HD22	0.60	1.73	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ILE:HG13	1:A:48:LEU:HD12	0.59	1.74	12	1
1:A:4:ILE:HB	1:A:8:VAL:HB	0.59	1.75	15	4
1:A:39:LEU:HD21	1:A:72:ILE:HB	0.59	1.74	14	8
1:A:6:ARG:HG2	1:A:7:THR:H	0.59	1.57	5	1
1:A:88:ILE:O	1:A:91:LEU:HG	0.58	1.97	14	18
1:A:50:GLU:HA	1:A:53:LYS:HB3	0.57	1.75	5	4
1:A:61:HIS:HB3	1:A:63:LEU:HD23	0.57	1.77	5	1
1:A:6:ARG:HG3	1:A:7:THR:H	0.57	1.59	7	1
1:A:136:ARG:HD2	1:A:136:ARG:O	0.56	1.99	13	1
1:A:65:SER:HB2	1:A:71:ILE:HB	0.56	1.76	6	1
1:A:132:ARG:HE	1:A:132:ARG:HA	0.54	1.62	11	1
1:A:86:ALA:O	1:A:90:ARG:HD3	0.54	2.03	18	3
1:A:52:TYR:O	1:A:56:LEU:HG	0.53	2.03	16	3
1:A:93:ALA:O	1:A:97:GLU:HG2	0.53	2.04	17	5
1:A:36:ALA:HB2	1:A:75:GLN:HB3	0.52	1.81	10	1
1:A:20:ILE:HB	1:A:36:ALA:HB3	0.52	1.81	3	1
1:A:43:ILE:HG13	1:A:56:LEU:HD13	0.52	1.80	16	1
1:A:92:VAL:O	1:A:96:LYS:HG3	0.51	2.05	2	1
1:A:61:HIS:CD2	1:A:97:GLU:HB3	0.51	2.40	5	1
1:A:20:ILE:CG1	1:A:38:HIS:HB2	0.51	2.36	2	3
1:A:90:ARG:O	1:A:94:VAL:HG23	0.51	2.06	16	6
1:A:74:ALA:HB2	1:A:87:ALA:HB2	0.51	1.82	13	2
1:A:5:SER:O	1:A:6:ARG:HB2	0.50	2.07	8	5
1:A:42:ASP:HB3	1:A:69:VAL:CB	0.49	2.35	5	1
1:A:76:GLU:HB2	1:A:82:LEU:HD11	0.49	1.82	16	1
1:A:43:ILE:HA	1:A:48:LEU:HD12	0.49	1.84	6	1
1:A:85:GLU:HG3	1:A:86:ALA:N	0.49	2.22	9	1
1:A:37:ILE:HD11	1:A:80:GLN:HE21	0.49	1.67	16	1
1:A:16:GLU:O	1:A:39:LEU:HA	0.48	2.09	5	2
1:A:6:ARG:HG2	1:A:7:THR:N	0.48	2.24	5	1
1:A:94:VAL:HA	1:A:97:GLU:HG2	0.47	1.86	10	1
1:A:50:GLU:O	1:A:54:GLN:HG2	0.47	2.09	17	6
1:A:50:GLU:CD	1:A:50:GLU:H	0.47	2.13	15	1
1:A:43:ILE:HG21	1:A:53:LYS:HG3	0.47	1.87	17	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.46	2.25	5	1
1:A:1:MET:HA	1:A:12:ASP:HB2	0.46	1.86	16	2
1:A:77:PHE:HB3	1:A:82:LEU:HD21	0.46	1.87	4	1
1:A:141:LEU:H	1:A:141:LEU:HD23	0.46	1.70	16	1
1:A:129:LYS:HE3	1:A:131:LEU:HD23	0.45	1.86	1	1
1:A:72:ILE:HG23	1:A:90:ARG:HH11	0.45	1.72	16	1
1:A:63:LEU:HG	1:A:94:VAL:HG22	0.45	1.87	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:VAL:HA	1:A:97:GLU:CG	0.45	2.42	10	1
1:A:55:ARG:HD2	1:A:98:LEU:O	0.44	2.11	2	1
1:A:65:SER:HB2	1:A:71:ILE:HD13	0.44	1.89	20	1
1:A:40:ARG:HA	1:A:70:ILE:O	0.44	2.12	2	1
1:A:39:LEU:CD2	1:A:72:ILE:HB	0.44	2.43	6	1
1:A:20:ILE:HG12	1:A:38:HIS:HB2	0.44	1.87	15	2
1:A:80:GLN:O	1:A:84:ARG:HG3	0.44	2.13	19	2
1:A:20:ILE:HD12	1:A:20:ILE:H	0.44	1.72	10	1
1:A:39:LEU:H	1:A:39:LEU:HD23	0.44	1.73	16	1
1:A:72:ILE:HG13	1:A:91:LEU:HB3	0.44	1.90	7	1
1:A:134:LYS:HD2	1:A:134:LYS:O	0.44	2.12	11	1
1:A:36:ALA:CB	1:A:75:GLN:HB3	0.44	2.43	10	3
1:A:86:ALA:O	1:A:90:ARG:HG2	0.44	2.12	2	1
1:A:56:LEU:HD23	1:A:98:LEU:HG	0.44	1.89	5	1
1:A:4:ILE:HB	1:A:8:VAL:O	0.44	2.12	6	3
1:A:94:VAL:HA	1:A:97:GLU:OE1	0.44	2.12	14	1
1:A:65:SER:CB	1:A:71:ILE:HD13	0.43	2.43	20	2
1:A:55:ARG:HD3	1:A:98:LEU:O	0.43	2.13	13	1
1:A:37:ILE:HD11	1:A:80:GLN:HB3	0.43	1.91	18	1
1:A:82:LEU:O	1:A:85:GLU:HG3	0.43	2.13	14	1
1:A:86:ALA:O	1:A:90:ARG:HB2	0.43	2.14	3	1
1:A:6:ARG:HA	1:A:6:ARG:NE	0.43	2.29	9	1
1:A:16:GLU:HB2	1:A:40:ARG:HB2	0.42	1.91	12	1
1:A:83:ASN:HD22	1:A:83:ASN:N	0.42	2.12	11	1
1:A:44:ARG:HB2	1:A:68:GLY:HA3	0.42	1.91	14	1
1:A:137:ARG:HE	1:A:137:ARG:HA	0.42	1.75	2	1
1:A:76:GLU:HB3	1:A:83:ASN:HD21	0.42	1.74	3	1
1:A:75:GLN:HG3	1:A:75:GLN:O	0.42	2.14	9	1
1:A:61:HIS:O	1:A:62:HIS:HB2	0.42	2.15	12	1
1:A:79:SER:HB3	1:A:82:LEU:HD23	0.42	1.91	18	1
1:A:79:SER:O	1:A:82:LEU:HG	0.42	2.15	12	1
1:A:64:ILE:HD13	1:A:70:ILE:CG2	0.42	2.45	16	1
1:A:64:ILE:HD13	1:A:70:ILE:HG12	0.42	1.91	10	1
1:A:131:LEU:O	1:A:132:ARG:HB2	0.41	2.15	7	1
1:A:2:ILE:HB	1:A:10:ILE:HB	0.41	1.92	11	2
1:A:18:THR:O	1:A:38:HIS:HB3	0.41	2.15	16	1
1:A:6:ARG:O	1:A:7:THR:HG22	0.41	2.15	19	1
1:A:63:LEU:HB3	1:A:70:ILE:HG23	0.41	1.92	2	1
1:A:2:ILE:HD12	1:A:2:ILE:N	0.41	2.31	13	1
1:A:55:ARG:HA	1:A:58:THR:OG1	0.41	2.15	13	1
1:A:94:VAL:O	1:A:98:LEU:HD13	0.41	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:82:LEU:HA	1:A:85:GLU:CG	0.41	2.45	19	2
1:A:63:LEU:HD12	1:A:94:VAL:HG21	0.41	1.92	9	1
1:A:136:ARG:NE	1:A:136:ARG:HA	0.41	2.31	10	1
1:A:20:ILE:HD11	1:A:38:HIS:HB2	0.41	1.92	14	1
1:A:76:GLU:HG2	1:A:77:PHE:CD2	0.41	2.51	13	1
1:A:56:LEU:HA	1:A:98:LEU:CD2	0.41	2.46	16	1
1:A:132:ARG:HD2	1:A:132:ARG:C	0.41	2.36	20	1
1:A:20:ILE:HD12	1:A:36:ALA:HB3	0.40	1.92	2	1
1:A:43:ILE:HG21	1:A:57:LEU:HD21	0.40	1.91	15	1
1:A:6:ARG:CG	1:A:7:THR:H	0.40	2.28	5	1
1:A:5:SER:O	1:A:6:ARG:HB3	0.40	2.16	6	1
1:A:4:ILE:HG22	1:A:5:SER:N	0.40	2.32	3	1
1:A:93:ALA:HA	1:A:96:LYS:HG2	0.40	1.93	8	1
1:A:72:ILE:N	1:A:72:ILE:HD12	0.40	2.32	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/148 (71%)	90±4 (86±4%)	13±4 (12±4%)	2±1 (2±1%)	9	52
All	All	2100/2960 (71%)	1810 (86%)	252 (12%)	38 (2%)	9	52

All 17 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	66	ASP	9
1	A	6	ARG	5
1	A	7	THR	4
1	A	77	PHE	4
1	A	133	GLY	2
1	A	46	SER	2
1	A	60	SER	2
1	A	47	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	68	GLY	1
1	A	59	ALA	1
1	A	78	ARG	1
1	A	129	LYS	1
1	A	132	ARG	1
1	A	126	SER	1
1	A	62	HIS	1
1	A	128	VAL	1
1	A	79	SER	1

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	90/124 (73%)	85±2 (95±2%)	5±2 (5±2%)	21	73
All	All	1800/2480 (73%)	1702 (95%)	98 (5%)	21	73

All 36 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	18	THR	17
1	A	61	HIS	6
1	A	142	GLU	6
1	A	80	GLN	5
1	A	82	LEU	5
1	A	21	ARG	4
1	A	50	GLU	3
1	A	75	GLN	3
1	A	83	ASN	3
1	A	90	ARG	3
1	A	73	LYS	3
1	A	134	LYS	3
1	A	96	LYS	3
1	A	6	ARG	2
1	A	53	LYS	2
1	A	40	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	44	ARG	2
1	A	81	GLU	2
1	A	7	THR	2
1	A	136	ARG	2
1	A	85	GLU	2
1	A	131	LEU	2
1	A	78	ARG	2
1	A	132	ARG	2
1	A	54	GLN	1
1	A	14	GLU	1
1	A	52	TYR	1
1	A	12	ASP	1
1	A	66	ASP	1
1	A	145	HIS	1
1	A	129	LYS	1
1	A	141	LEU	1
1	A	42	ASP	1
1	A	138	PRO	1
1	A	139	LEU	1
1	A	76	GLU	1

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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 87% for the well-defined parts and 80% 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	1702
Number of shifts mapped to atoms	1702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	136	-0.05 ± 0.05	None needed (< 0.5 ppm)
$^{13}C_\beta$	130	0.16 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	132	-0.08 ± 0.10	None needed (< 0.5 ppm)
^{15}N	132	-0.42 ± 0.30	None needed (< 0.5 ppm)

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 87%, i.e. 1339 atoms were assigned a chemical shift out of a possible 1541. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	510/529 (96%)	206/213 (97%)	204/212 (96%)	100/104 (96%)
Sidechain	795/926 (86%)	545/606 (90%)	245/277 (88%)	5/43 (12%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	34/86 (40%)	21/42 (50%)	13/32 (41%)	0/12 (0%)
Overall	1339/1541 (87%)	772/861 (90%)	462/521 (89%)	105/159 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1702 atoms were assigned a chemical shift out of a possible 2118. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	676/740 (91%)	276/299 (92%)	268/296 (91%)	132/145 (91%)
Sidechain	988/1260 (78%)	678/817 (83%)	303/372 (81%)	7/71 (10%)
Aromatic	38/118 (32%)	23/58 (40%)	15/40 (38%)	0/20 (0%)
Overall	1702/2118 (80%)	977/1174 (83%)	586/708 (83%)	139/236 (59%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	92	VAL	CG2	-5.65	13.71 − 28.88	-17.8
1	A	43	ILE	CB	55.39	28.63 − 48.45	8.5

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:
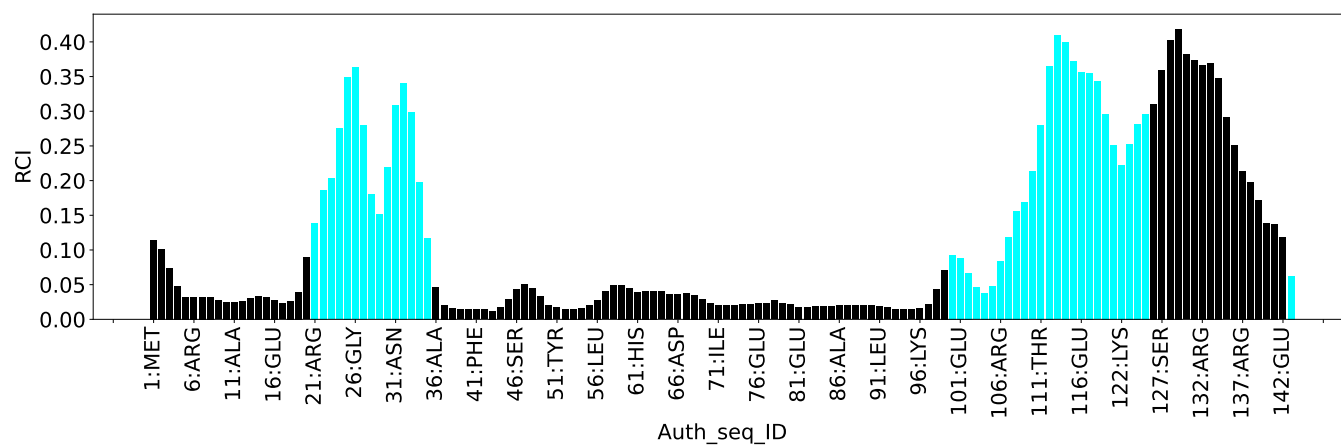
8 NMR restraints analysis ⓘ

8.1 Conformationally restricting restraints ⓘ

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1201
Intra-residue ($\lvert i\text{-}j\rvert$=0)	309
Sequential ($\lvert i\text{-}j\rvert$=1)	405
Medium range ($\lvert i\text{-}j\rvert$>1 and $\lvert i\text{-}j\rvert$<5)	180
Long range ($\lvert i\text{-}j\rvert$≥5)	307
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	331
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue[1]	2.1

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

8.2 Residual restraint violations ⓘ

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

8.2.1 Average number of distance violations per model ⓘ

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.5	0.2
0.2-0.5 (Medium)	0.9	0.43
>0.5 (Large)	None	None

8.2.2   Average number of dihedral-angle violations per model ⓘ

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)	10.8	9.91
10.0-20.0 (Medium)	2.7	19.68
>20.0 (Large)	3.0	100.11

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.

Restraints type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue (|i-j|=0)	309	25.7	14	4.5	1.2	0	0.0	0.0
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	296	24.6	14	4.7	1.2	0	0.0	0.0
Sidechain-Sidechain	9	0.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	405	33.7	22	5.4	1.8	0	0.0	0.0
Backbone-Backbone	134	11.2	11	8.2	0.9	0	0.0	0.0
Backbone-Sidechain	248	20.6	10	4.0	0.8	0	0.0	0.0
Sidechain-Sidechain	23	1.9	1	4.3	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	180	15.0	8	4.4	0.7	0	0.0	0.0
Backbone-Backbone	43	3.6	3	7.0	0.2	0	0.0	0.0
Backbone-Sidechain	83	6.9	4	4.8	0.3	0	0.0	0.0
Sidechain-Sidechain	54	4.5	1	1.9	0.1	0	0.0	0.0
Long range (|i-j|≥5)	307	25.6	5	1.6	0.4	0	0.0	0.0
Backbone-Backbone	19	1.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	99	8.2	2	2.0	0.2	0	0.0	0.0
Sidechain-Sidechain	189	15.7	3	1.6	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1201	100.0	49	4.1	4.1	0	0.0	0.0
Backbone-Backbone	200	16.7	14	7.0	1.2	0	0.0	0.0
Backbone-Sidechain	726	60.4	30	4.1	2.5	0	0.0	0.0
Sidechain-Sidechain	275	22.9	5	1.8	0.4	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 ⓘ
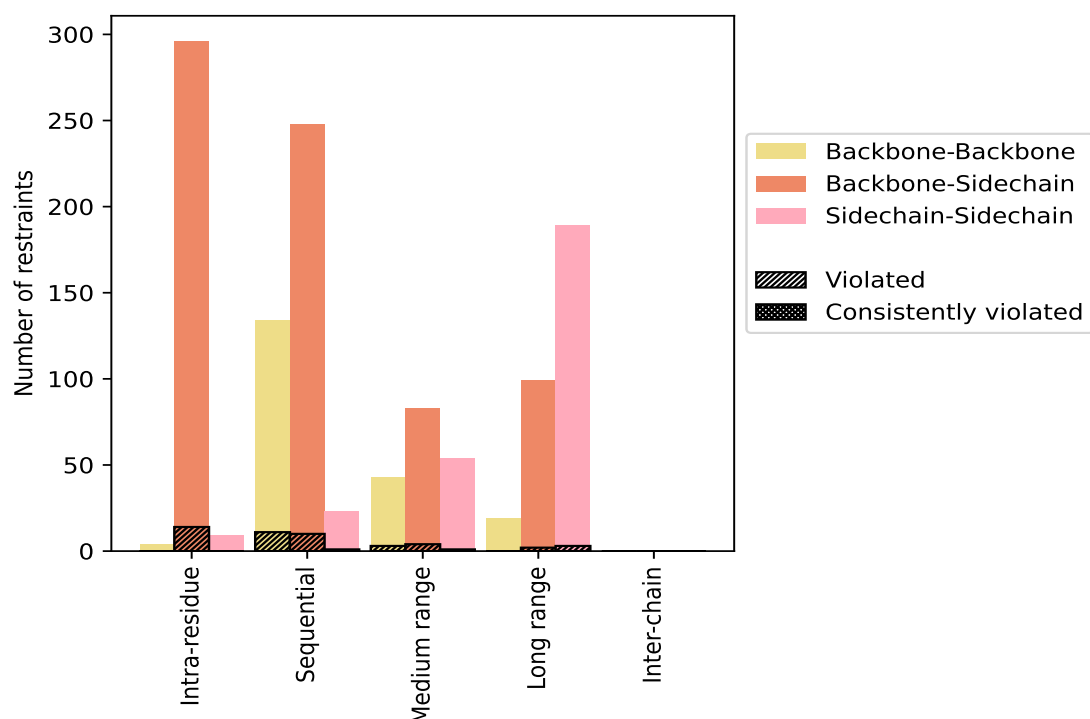
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2   Distance violation statistics for each model ⓘ

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	2	0	0	0	4	0.21	0.33	0.1	0.2
2	0	3	2	0	0	5	0.13	0.17	0.02	0.13
3	3	2	0	0	0	5	0.14	0.15	0.01	0.14
4	2	3	0	0	0	5	0.15	0.25	0.06	0.11
5	5	5	0	2	0	12	0.17	0.43	0.09	0.14
6	2	5	0	0	0	7	0.17	0.38	0.09	0.13
7	3	5	1	1	0	10	0.16	0.26	0.05	0.13
8	3	4	1	0	0	8	0.13	0.17	0.02	0.13
9	5	0	3	0	0	8	0.14	0.19	0.02	0.13
10	2	4	1	0	0	7	0.17	0.27	0.06	0.15

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	4	0	0	0	8	0.15	0.18	0.03	0.16
12	5	2	0	0	0	7	0.19	0.35	0.08	0.15
13	1	1	0	1	0	3	0.11	0.12	0.0	0.11
14	4	0	1	0	0	5	0.15	0.17	0.02	0.16
15	3	5	1	0	0	9	0.16	0.24	0.04	0.16
16	1	4	0	0	0	5	0.15	0.24	0.05	0.14
17	1	4	1	0	0	6	0.13	0.22	0.04	0.11
18	4	1	0	0	0	5	0.16	0.25	0.05	0.14
19	4	3	1	1	0	9	0.16	0.2	0.03	0.16
20	5	6	0	0	0	11	0.15	0.26	0.05	0.15

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

9.2.1　Bar graph : Distance Violation statistics for each model ⓘ
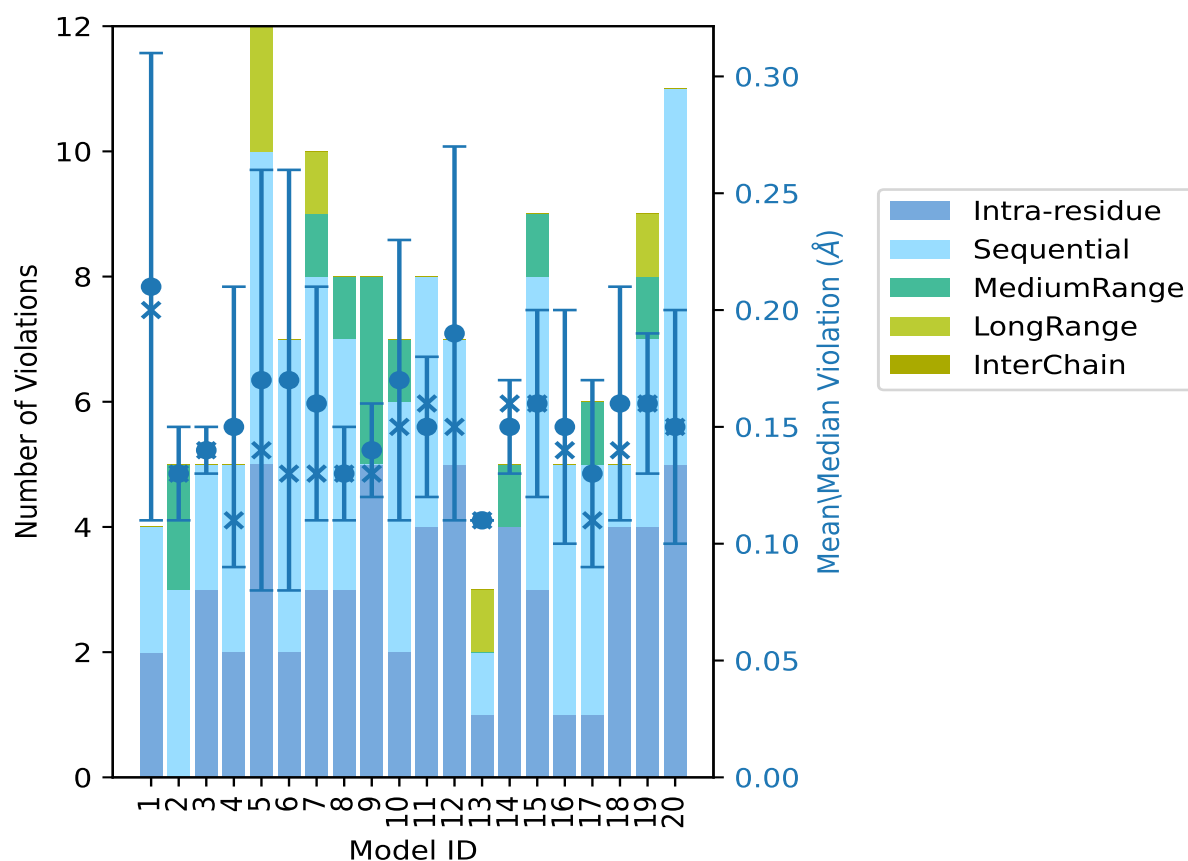
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis
on the right

9.3   Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1152(IR:295, SQ:383, MR:172, LR:302, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
2	10	6	5	0	23	1	5.0
2	4	1	0	0	7	2	10.0
3	0	0	0	0	3	3	15.0
3	3	1	0	0	7	4	20.0
0	1	0	0	0	1	5	25.0
2	2	0	0	0	4	6	30.0
0	1	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
1	1	0	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
1	0	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ
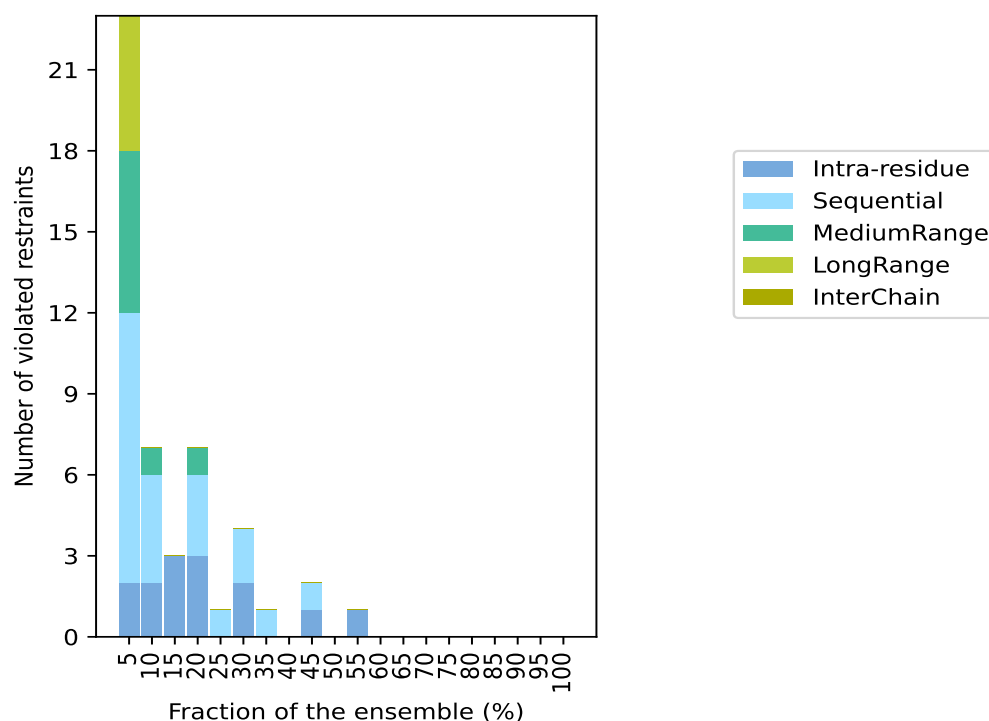
9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
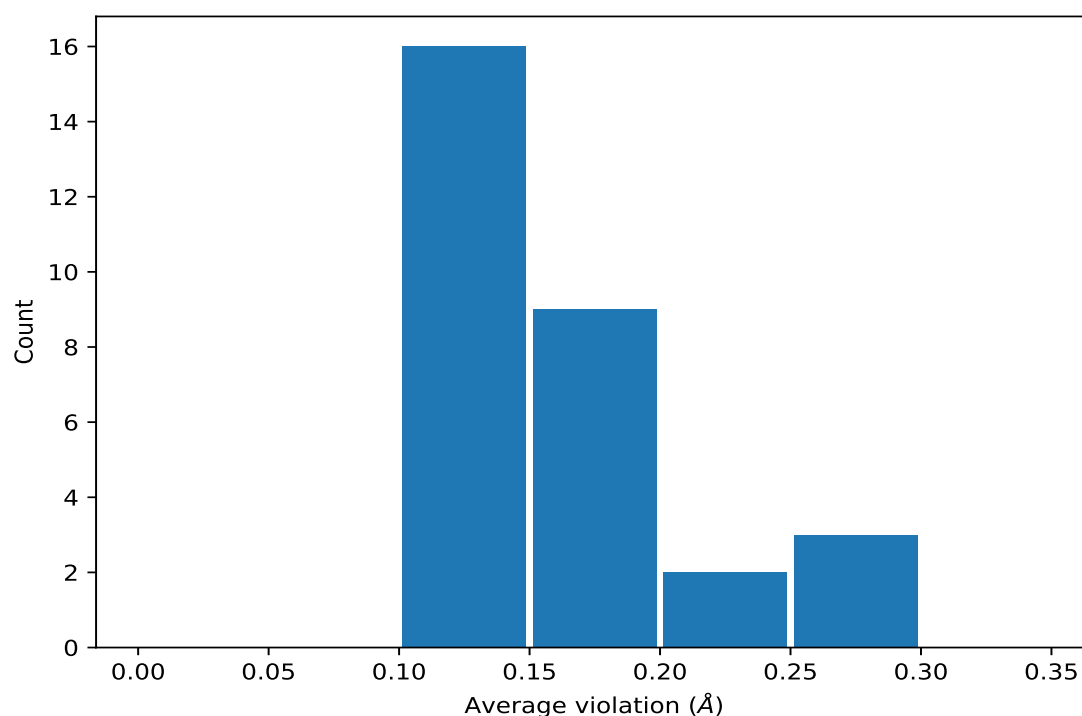
9.4.2 Table: Most violated distance restraints ⓘ

The following table provides the mean and the standard deviation of the 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[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	11	0.11	0.01	0.11
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	9	0.2	0.04	0.19
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	9	0.18	0.05	0.17
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	7	0.17	0.03	0.17
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	6	0.19	0.03	0.18
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	6	0.15	0.01	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	6	0.15	0.01	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	6	0.15	0.01	0.15
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	6	0.14	0.03	0.13
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	6	0.14	0.0	0.14
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	5	0.13	0.01	0.13
(1,330)	1:82:A:LEU:H	1:82:A:LEU:HG	4	0.26	0.08	0.24
(1,541)	1:82:A:LEU:HA	1:85:A:GLU:HB2	4	0.15	0.02	0.15
(1,499)	1:20:A:ILE:HB	1:21:A:ARG:H	4	0.15	0.04	0.14
(1,471)	1:18:A:THR:H	1:18:A:THR:HB	4	0.13	0.02	0.13
(1,484)	1:85:A:GLU:H	1:85:A:GLU:HB2	4	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,79)	1:64:A:ILE:HB	1:65:A:SER:H	4	0.12	0.01	0.12
(1,498)	1:18:A:THR:HB	1:19:A:ALA:H	4	0.11	0.01	0.11
(1,181)	1:81:A:GLU:H	1:81:A:GLU:HB3	3	0.29	0.04	0.26
(1,175)	1:69:A:VAL:H	1:69:A:VAL:HB	3	0.15	0.01	0.14
(1,566)	1:98:A:LEU:H	1:98:A:LEU:HG	3	0.11	0.0	0.11
(1,323)	1:63:A:LEU:H	1:63:A:LEU:HG	2	0.27	0.16	0.27
(1,335)	1:96:A:LYS:H	1:96:A:LYS:HG3	2	0.21	0.04	0.21
(1,124)	1:108:A:THR:HA	1:109:A:ARG:H	2	0.14	0.02	0.14
(1,255)	1:65:A:SER:H	1:69:A:VAL:H	2	0.14	0.01	0.14
(1,33)	1:30:A:VAL:HA	1:31:A:ASN:H	2	0.11	0.0	0.11
(1,224)	1:67:A:ASP:H	1:68:A:GLY:H	2	0.11	0.01	0.11
(1,367)	1:43:A:ILE:HD11	1:44:A:ARG:H	2	0.11	0.0	0.11
(1,367)	1:43:A:ILE:HD12	1:44:A:ARG:H	2	0.11	0.0	0.11
(1,367)	1:43:A:ILE:HD13	1:44:A:ARG:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
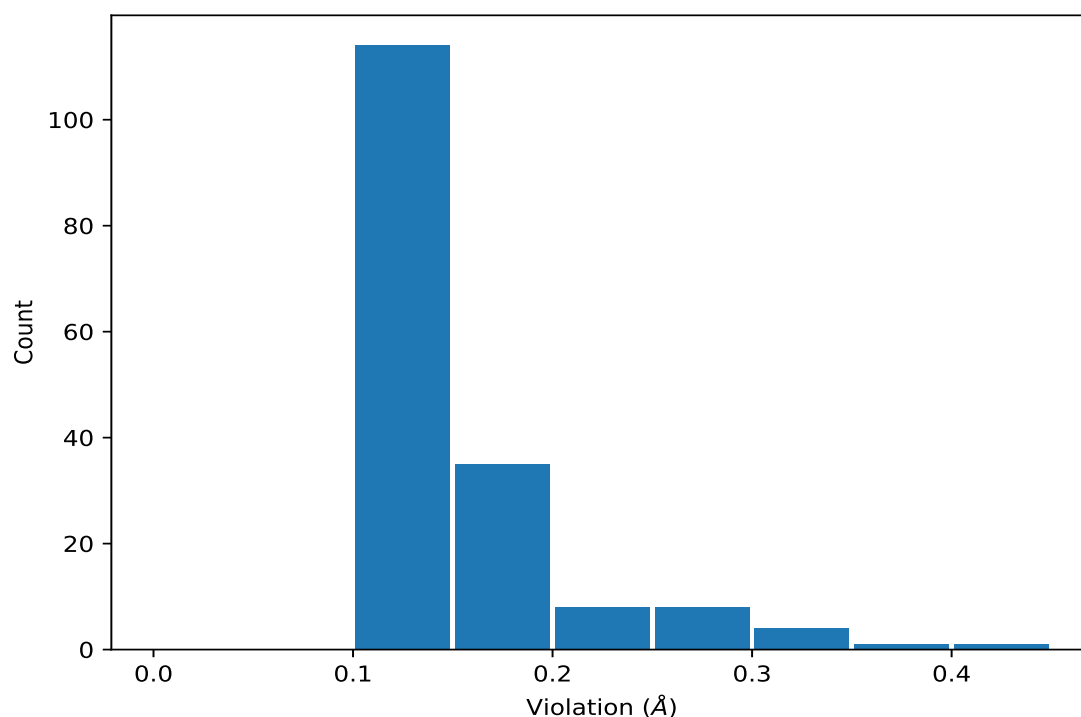
9.5.2   Table : All distance violations ⓘ

The following table 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)
(1,323)	1:63:A:LEU:H	1:63:A:LEU:HG	5	0.43
(1,330)	1:82:A:LEU:H	1:82:A:LEU:HG	6	0.38
(1,181)	1:81:A:GLU:H	1:81:A:GLU:HB3	12	0.35
(1,617)	1:6:A:ARG:HB2	1:7:A:THR:HG21	1	0.33
(1,617)	1:6:A:ARG:HB2	1:7:A:THR:HG22	1	0.33
(1,617)	1:6:A:ARG:HB2	1:7:A:THR:HG23	1	0.33
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	12	0.29
(1,330)	1:82:A:LEU:H	1:82:A:LEU:HG	1	0.29
(1,542)	1:94:A:VAL:HA	1:97:A:GLU:HB2	10	0.27
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	7	0.26
(1,181)	1:81:A:GLU:H	1:81:A:GLU:HB3	20	0.26
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	7	0.25
(1,335)	1:96:A:LYS:H	1:96:A:LYS:HG3	18	0.25
(1,181)	1:81:A:GLU:H	1:81:A:GLU:HB3	4	0.25
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	10	0.24
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	15	0.24
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	16	0.24
(1,499)	1:20:A:ILE:HB	1:21:A:ARG:H	15	0.22
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	17	0.22
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	5	0.21
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	20	0.21
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	19	0.2
(1,541)	1:82:A:LEU:HA	1:85:A:GLU:HB2	19	0.19
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	5	0.19
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	9	0.19
(1,330)	1:82:A:LEU:H	1:82:A:LEU:HG	5	0.19
(1,327)	1:75:A:GLN:H	1:75:A:GLN:HG2	7	0.19
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	11	0.18
(1,330)	1:82:A:LEU:H	1:82:A:LEU:HG	11	0.18
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	15	0.18
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	16	0.18
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	4	0.18
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	20	0.18
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	14	0.17
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	15	0.17
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	18	0.17
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	18	0.17
(1,335)	1:96:A:LYS:H	1:96:A:LYS:HG3	14	0.17
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	2	0.17
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	6	0.17
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	12	0.17
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	8	0.17
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	20	0.17
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	19	0.17
(1,541)	1:82:A:LEU:HA	1:85:A:GLU:HB2	14	0.16
(1,482)	1:76:A:GLU:H	1:76:A:GLU:HB3	19	0.16
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	19	0.16
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	19	0.16
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	19	0.16
(1,374)	1:71:A:ILE:HG21	1:72:A:ILE:H	5	0.16
(1,374)	1:71:A:ILE:HG22	1:72:A:ILE:H	5	0.16
(1,374)	1:71:A:ILE:HG23	1:72:A:ILE:H	5	0.16
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	11	0.16
(1,216)	1:46:A:SER:H	1:47:A:GLY:H	10	0.16
(1,175)	1:69:A:VAL:H	1:69:A:VAL:HB	15	0.16
(1,124)	1:108:A:THR:HA	1:109:A:ARG:H	11	0.16
(1,533)	1:93:A:ALA:HA	1:96:A:LYS:HB2	8	0.15
(1,499)	1:20:A:ILE:HB	1:21:A:ARG:H	10	0.15
(1,471)	1:18:A:THR:H	1:18:A:THR:HB	20	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	12	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	12	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	12	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	20	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	20	0.15
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	20	0.15
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	2	0.15
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	19	0.15
(1,95)	1:74:A:ALA:H	1:75:A:GLN:H	6	0.15
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	15	0.15
(1,54)	1:46:A:SER:HA	1:47:A:GLY:H	11	0.15
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	3	0.15
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	12	0.14
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	18	0.14
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	19	0.14
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	20	0.14
(1,471)	1:18:A:THR:H	1:18:A:THR:HB	3	0.14
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	5	0.14
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	5	0.14
(1,417)	1:58:A:THR:H	1:58:A:THR:HG21	9	0.14
(1,417)	1:58:A:THR:H	1:58:A:THR:HG22	9	0.14
(1,417)	1:58:A:THR:H	1:58:A:THR:HG23	9	0.14
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	8	0.14
(1,255)	1:65:A:SER:H	1:69:A:VAL:H	9	0.14
(1,228)	1:75:A:GLN:H	1:76:A:GLU:H	3	0.14
(1,175)	1:69:A:VAL:H	1:69:A:VAL:HB	3	0.14
(1,175)	1:69:A:VAL:H	1:69:A:VAL:HB	8	0.14
(1,147)	1:30:A:VAL:H	1:30:A:VAL:HB	14	0.14
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	16	0.14
(1,668)	1:40:A:ARG:HA	1:71:A:ILE:HG21	5	0.13
(1,668)	1:40:A:ARG:HA	1:71:A:ILE:HG22	5	0.13
(1,668)	1:40:A:ARG:HA	1:71:A:ILE:HG23	5	0.13
(1,649)	1:59:A:ALA:HB1	1:61:A:HIS:HD2	9	0.13
(1,649)	1:59:A:ALA:HB2	1:61:A:HIS:HD2	9	0.13
(1,649)	1:59:A:ALA:HB3	1:61:A:HIS:HD2	9	0.13
(1,541)	1:82:A:LEU:HA	1:85:A:GLU:HB2	7	0.13
(1,541)	1:82:A:LEU:HA	1:85:A:GLU:HB2	9	0.13
(1,526)	1:82:A:LEU:HA	1:85:A:GLU:HB3	2	0.13
(1,499)	1:20:A:ILE:HB	1:21:A:ARG:H	11	0.13
(1,498)	1:18:A:THR:HB	1:19:A:ALA:H	7	0.13
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	5	0.13
(1,477)	1:58:A:THR:HA	1:58:A:THR:HB	9	0.13
(1,299)	1:62:A:HIS:HD2	1:63:A:LEU:H	6	0.13
(1,255)	1:65:A:SER:H	1:69:A:VAL:H	15	0.13
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	10	0.13
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	20	0.13
(1,79)	1:64:A:ILE:HB	1:65:A:SER:H	12	0.13
(1,72)	1:60:A:SER:HA	1:61:A:HIS:H	7	0.13
(1,660)	1:40:A:ARG:HG2	1:69:A:VAL:HG21	13	0.12
(1,660)	1:40:A:ARG:HG2	1:69:A:VAL:HG22	13	0.12
(1,660)	1:40:A:ARG:HG2	1:69:A:VAL:HG23	13	0.12
(1,498)	1:18:A:THR:HB	1:19:A:ALA:H	15	0.12
(1,484)	1:85:A:GLU:H	1:85:A:GLU:HB2	7	0.12
(1,484)	1:85:A:GLU:H	1:85:A:GLU:HB2	9	0.12
(1,484)	1:85:A:GLU:H	1:85:A:GLU:HB2	19	0.12
(1,471)	1:18:A:THR:H	1:18:A:THR:HB	9	0.12
(1,224)	1:67:A:ASP:H	1:68:A:GLY:H	8	0.12
(1,124)	1:108:A:THR:HA	1:109:A:ARG:H	10	0.12
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	7	0.12
(1,79)	1:64:A:ILE:HB	1:65:A:SER:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:29:A:HIS:HA	1:30:A:VAL:H	6	0.12
(1,763)	1:16:A:GLU:HB2	1:40:A:ARG:H	7	0.11
(1,763)	1:16:A:GLU:HB3	1:40:A:ARG:H	7	0.11
(1,700)	1:61:A:HIS:HD2	1:94:A:VAL:HG21	19	0.11
(1,700)	1:61:A:HIS:HD2	1:94:A:VAL:HG22	19	0.11
(1,700)	1:61:A:HIS:HD2	1:94:A:VAL:HG23	19	0.11
(1,566)	1:98:A:LEU:H	1:98:A:LEU:HG	1	0.11
(1,566)	1:98:A:LEU:H	1:98:A:LEU:HG	4	0.11
(1,566)	1:98:A:LEU:H	1:98:A:LEU:HG	8	0.11
(1,527)	1:86:A:ALA:HA	1:90:A:ARG:H	17	0.11
(1,499)	1:20:A:ILE:HB	1:21:A:ARG:H	7	0.11
(1,484)	1:85:A:GLU:H	1:85:A:GLU:HB2	14	0.11
(1,367)	1:43:A:ILE:HD11	1:44:A:ARG:H	10	0.11
(1,367)	1:43:A:ILE:HD12	1:44:A:ARG:H	10	0.11
(1,367)	1:43:A:ILE:HD13	1:44:A:ARG:H	10	0.11
(1,323)	1:63:A:LEU:H	1:63:A:LEU:HG	8	0.11
(1,212)	1:36:A:ALA:H	1:37:A:ILE:H	13	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	3	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	6	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	11	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	12	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	13	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	15	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	16	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	17	0.11
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	18	0.11
(1,105)	1:84:A:ARG:HB2	1:85:A:GLU:H	5	0.11
(1,100)	1:80:A:GLN:HB2	1:81:A:GLU:H	4	0.11
(1,100)	1:80:A:GLN:HB3	1:81:A:GLU:H	4	0.11
(1,83)	1:67:A:ASP:HA	1:68:A:GLY:H	17	0.11
(1,79)	1:64:A:ILE:HB	1:65:A:SER:H	1	0.11
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	4	0.11
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	8	0.11
(1,33)	1:30:A:VAL:HA	1:31:A:ASN:H	17	0.11
(1,33)	1:30:A:VAL:HA	1:31:A:ASN:H	18	0.11
(1,667)	1:38:A:HIS:HD2	1:71:A:ILE:HG21	5	0.1
(1,667)	1:38:A:HIS:HD2	1:71:A:ILE:HG22	5	0.1
(1,667)	1:38:A:HIS:HD2	1:71:A:ILE:HG23	5	0.1
(1,498)	1:18:A:THR:HB	1:19:A:ALA:H	6	0.1
(1,498)	1:18:A:THR:HB	1:19:A:ALA:H	17	0.1
(1,471)	1:18:A:THR:H	1:18:A:THR:HB	11	0.1
(1,367)	1:43:A:ILE:HD11	1:44:A:ARG:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:43:A:ILE:HD12	1:44:A:ARG:H	20	0.1
(1,367)	1:43:A:ILE:HD13	1:44:A:ARG:H	20	0.1
(1,259)	1:79:A:SER:HA	1:82:A:LEU:H	2	0.1
(1,224)	1:67:A:ASP:H	1:68:A:GLY:H	5	0.1
(1,185)	1:85:A:GLU:H	1:85:A:GLU:HB3	20	0.1
(1,79)	1:64:A:ILE:HB	1:65:A:SER:H	20	0.1
(1,44)	1:38:A:HIS:HB2	1:39:A:LEU:H	16	0.1
(1,34)	1:30:A:VAL:HB	1:31:A:ASN:H	5	0.1

10 Dihedral-angle violation analysis ⓘ

10.1 Summary of dihedral-angle violations ⓘ

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

Angle type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
CHI2	43	13.0	8	18.6	2.4	1	2.3	0.3
PHI	103	31.1	11	10.7	3.3	0	0.0	0.0
CHI1	73	22.1	15	20.5	4.5	2	2.7	0.6
PSI	100	30.2	27	27.0	8.2	0	0.0	0.0
CHI21	12	3.6	2	16.7	0.6	1	8.3	0.3
Total	331	100.0	63	19.0	19.0	4	1.2	1.2

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations ⓘ
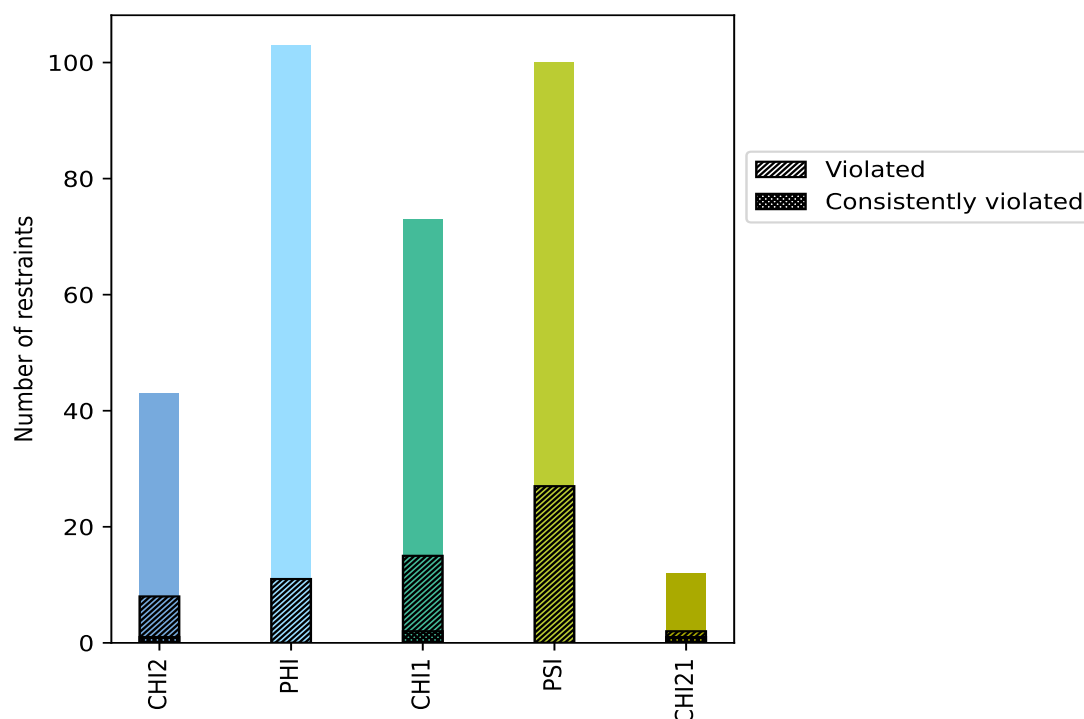
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)
	CHI2	PHI	CHI1	PSI	CHI21	Total				
1	3	1	5	4	2	15	14.68	51.08	16.95	6.54
2	2	2	6	5	2	17	9.03	49.84	12.18	3.54
3	4	2	9	3	2	20	11.37	49.13	12.21	6.41
4	1	1	7	5	2	16	12.37	48.95	12.88	7.81
5	3	2	7	5	2	19	11.96	62.78	17.84	4.35
6	4	2	6	4	2	18	14.24	49.44	17.3	4.82
7	3	1	7	7	2	20	14.93	100.11	23.28	5.62
8	2	0	6	2	2	12	14.95	51.76	15.09	8.35
9	1	2	8	3	2	16	12.42	67.71	18.66	3.89
10	3	0	6	3	2	14	14.03	49.16	16.78	5.68
11	3	1	5	3	2	14	8.61	48.88	11.97	4.5
12	2	1	7	7	2	19	14.47	76.85	20.63	4.38
13	4	1	6	5	2	18	11.83	50.84	14.63	4.24
14	2	2	6	3	2	15	11.3	49.44	15.8	4.31
15	2	2	6	5	2	17	6.71	49.81	11.1	3.01
16	2	3	5	1	2	13	14.21	49.79	13.37	13.19
17	4	0	6	5	2	17	11.36	48.21	13.68	5.5
18	2	0	8	8	2	20	13.79	71.35	17.68	6.09
19	3	1	6	3	1	14	15.59	75.24	20.76	6.01
20	2	1	7	4	2	16	15.76	66.79	19.66	5.57

10.2.1　Bar graph : Dihedral violation statistics for each model ⓘ
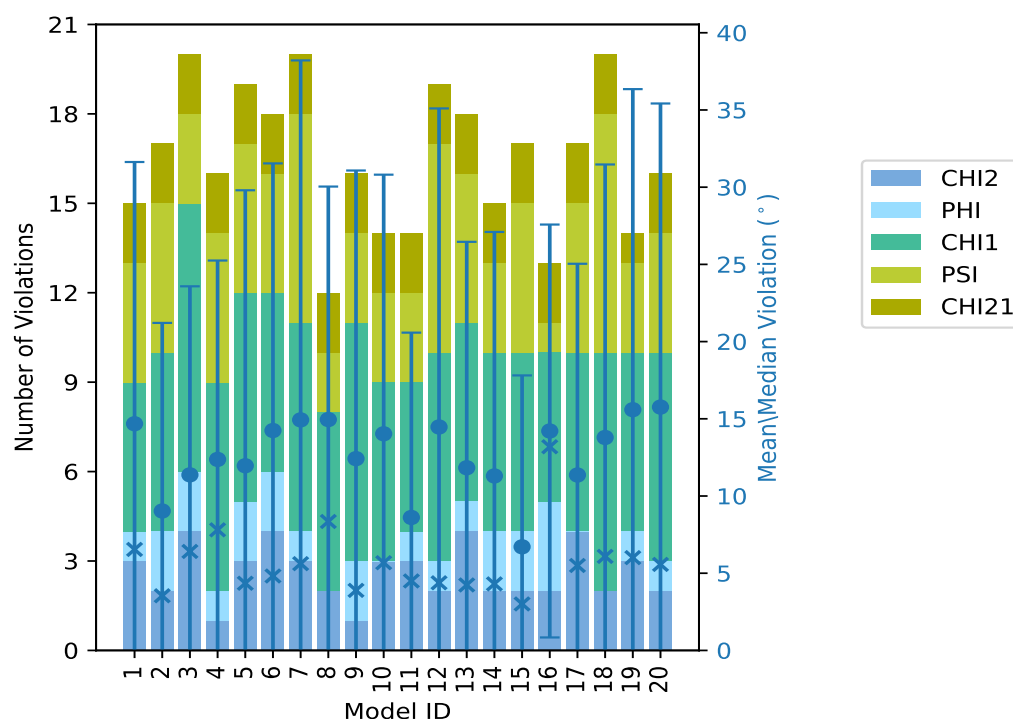
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3　Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints						Fraction of the ensemble	
CHI2	PHI	CHI1	PSI	CHI21	Total	Count[1]	%
2	6	3	12	0	23	1	5.0
2	2	1	6	0	11	2	10.0
0	0	2	1	0	3	3	15.0
1	1	1	0	0	3	4	20.0
0	1	0	2	0	3	5	25.0
0	1	1	4	0	6	6	30.0
0	0	0	0	0	0	7	35.0
1	0	0	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	2	0	0	2	10	50.0
0	0	1	1	0	2	11	55.0

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| Number of violated restraints | | | | | | Fraction of the ensemble | |
CHI2	PHI	CHI1	PSI	CHI21	Total	Count[1]	%
0	0	0	0	0	0	12	60.0
0	0	0	1	0	1	13	65.0
1	0	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	0	1	0	1	2	19	95.0
1	0	2	0	1	4	20	100.0

[1] Number of models with violations

10.3.1   Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ
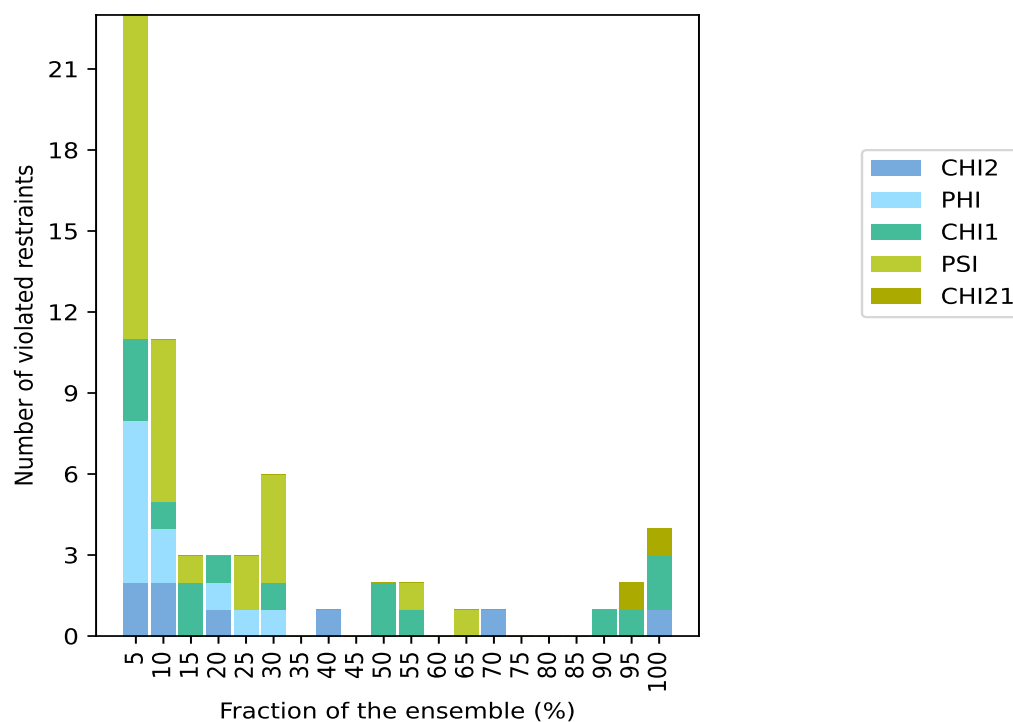
10.4   Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1   Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble

10.4.2   Table: Most violated dihedral-angle restraints (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.

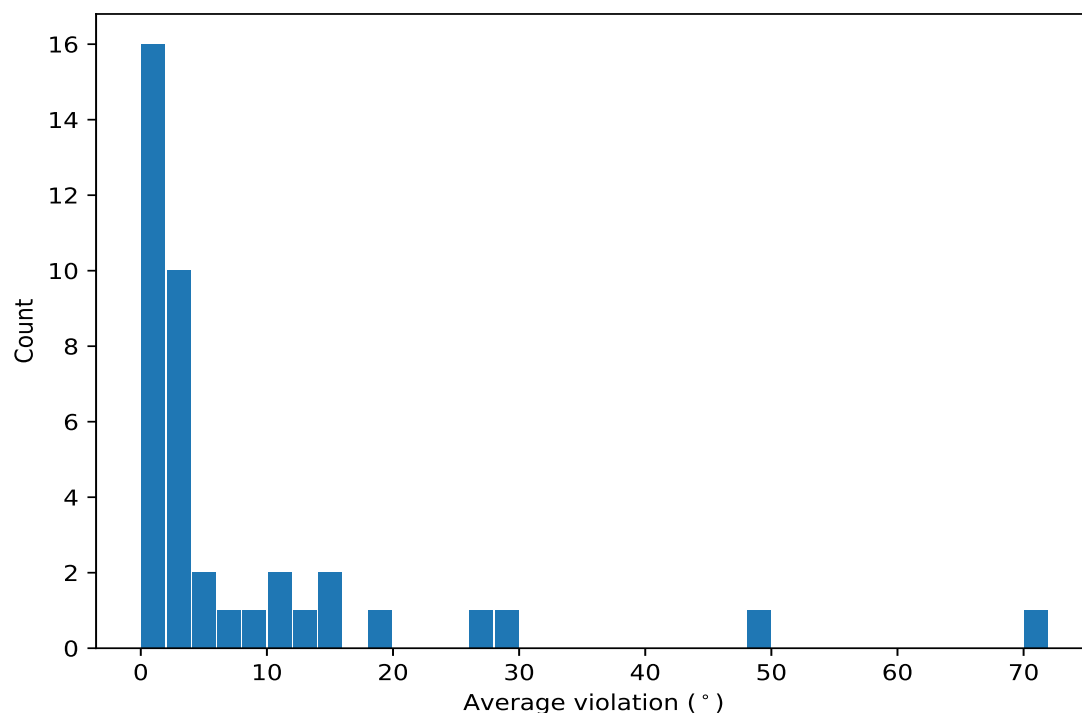| Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Media
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	20	49.7	0.97	49.44
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	20	15.67	3.72	15.38
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	20	10.33	4.12	10.55
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	20	5.11	1.13	5.17
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	19	27.59	14.56	20.14
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	19	6.42	3.47	5.76
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	18	19.11	9.42	18.5
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	14	3.76	1.81	3.8
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	13	2.5	1.17	2.17
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	11	12.4	14.28	5.59
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	11	2.09	0.74	2.2
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	10	28.62	9.08	29.01
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	10	9.63	4.39	8.8
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	8	5.5	2.07	4.96
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	6	70.12	4.9	69.53
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	6	2.59	0.71	2.8
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	6	2.12	0.91	2.0
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	6	2.07	0.69	1.96
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	6	1.98	0.79	1.9
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	6	1.33	0.26	1.27

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	5	1.82	0.52	1.53
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	5	1.68	0.48	1.37
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	5	1.58	0.37	1.57
(1,274)	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	1:75:A:GLN:CD	4	15.6	9.1	14.88
(1,309)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:CB	1:98:A:LEU:CG	4	3.66	2.13	3.08
(1,210)	1:47:A:GLY:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	4	1.39	0.26	1.28
(1,140)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:CB	1:18:A:THR:OG1	3	11.66	1.82	12.14
(1,33)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ASP:N	3	1.71	0.32	1.55
(1,138)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:CB	1:17:A:ILE:CG1	3	1.18	0.09	1.17
(1,228)	1:55:A:ARG:CA	1:55:A:ARG:CB	1:55:A:ARG:CG	1:55:A:ARG:CD	2	3.52	1.72	3.52
(1,128)	1:13:A:ASN:CA	1:13:A:ASN:CB	1:13:A:ASN:CG	1:13:A:ASN:OD1	2	2.97	1.81	2.97
(1,253)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:CB	1:64:A:ILE:CG1	2	2.36	0.4	2.36
(1,58)	1:72:A:ILE:C	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:C	2	1.93	0.68	1.93
(1,331)	1:105:A:ARG:N	1:105:A:ARG:CA	1:105:A:ARG:C	1:106:A:ARG:N	2	1.8	0.31	1.8
(1,163)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:HIS:N	2	1.62	0.16	1.62
(1,38)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	2	1.47	0.36	1.47
(1,213)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:PRO:N	2	1.4	0.3	1.4
(1,97)	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1:97:A:GLU:N	2	1.35	0.24	1.35
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:SER:N	2	1.32	0.12	1.32
(1,35)	1:42:A:ASP:N	1:42:A:ASP:CA	1:42:A:ASP:C	1:43:A:ILE:N	2	1.14	0.06	1.14

[1] Number of violated models, [2]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.
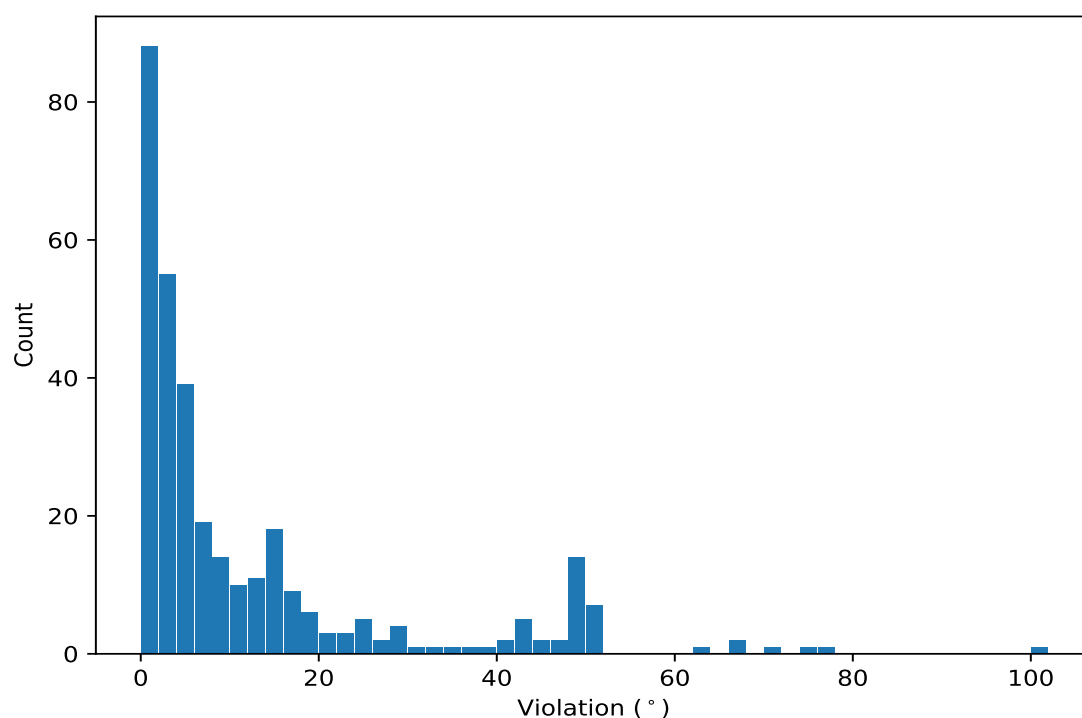
10.5.2 Table: All violated dihedral-angle restraints ⓘ

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 (°)
(1,273)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	7	100.11
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	12	76.85
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	19	75.24
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	18	71.35
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	9	67.71
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	20	66.79
(1,234)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:CB	1:58:A:THR:OG1	5	62.78
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	8	51.76
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	7	51.49
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	1	51.08
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	13	50.84
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	9	50.58
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	12	50.33
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	20	50.05
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	2	49.84
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	15	49.81
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	16	49.79
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	6	49.44
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	14	49.44
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	12	49.25
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	10	49.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	3	49.13
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	4	48.95
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	5	48.95
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	19	48.95
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	11	48.88
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	18	48.43
(1,300)	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1:88:A:ILE:CD1	17	48.21
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	6	47.46
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	10	46.49
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	1	45.83
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	20	44.72
(1,226)	1:54:A:GLN:CA	1:54:A:GLN:CB	1:54:A:GLN:CG	1:54:A:GLN:CD	6	43.42
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	1	42.72
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	13	42.7
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	5	42.58
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	14	42.13
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	17	41.42
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	6	40.22
(1,296)	1:84:A:ARG:CA	1:84:A:ARG:CB	1:84:A:ARG:CG	1:84:A:ARG:CD	10	39.12
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	8	37.62
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	14	34.44
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	3	33.45
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	7	31.86
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	13	29.8
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	4	29.76
(1,274)	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	1:75:A:GLN:CD	7	29.13
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	18	28.26
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	19	26.6
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	3	26.26
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	20	25.95
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	16	25.64
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	8	25.5
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	12	25.24
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	16	24.93
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	2	23.51
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	4	22.88
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1	22.75
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	4	20.84
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	18	20.24
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	18	20.14
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	9	19.68
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	16	19.1
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	16	19.0
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	13	18.91
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	6	18.33
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	17	18.27
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	2	17.59
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	4	17.42
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	10	17.37
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	17	17.32
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	17	17.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	4	16.85
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	6	16.75
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	3	16.69
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	8	16.38
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	19	15.87
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	7	15.85
(1,274)	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	1:75:A:GLN:CD	3	15.67
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	18	15.67
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	2	15.48
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	13	15.32
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	18	15.26
(1,276)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:CB	1:76:A:GLU:CG	17	14.89
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	5	14.89
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	19	14.83
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	18	14.82
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	3	14.72
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	16	14.64
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	11	14.53
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	18	14.15
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	13	14.1
(1,274)	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	1:75:A:GLN:CD	13	14.09
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	3	14.0
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	5	13.73
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	1	13.69
(1,140)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:CB	1:18:A:THR:OG1	3	13.61
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	8	13.33
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	16	13.19
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	2	13.01
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	12	12.68
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	11	12.67
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	7	12.53
(1,140)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:CB	1:18:A:THR:OG1	20	12.14
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	9	12.1
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	14	11.79
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	10	11.74
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	9	11.29
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	12	11.24
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	20	11.21
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	15	11.0
(1,188)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	20	10.97
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	1	10.88
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	6	10.71
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	11	10.39
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	12	9.91
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	9	9.81
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	8	9.81
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	7	9.67
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	4	9.63
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	7	9.61
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	1	9.29
(1,140)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:CB	1:18:A:THR:OG1	9	9.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	2	8.96
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	17	8.87
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	4	8.64
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	3	8.46
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	19	8.32
(1,197)	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	1:43:A:ILE:CD1	15	8.02
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	5	7.68
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	15	7.59
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	18	7.52
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	11	7.48
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	11	7.41
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	7	7.37
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	3	7.37
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	12	7.29
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	4	6.98
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	8	6.88
(1,309)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:CB	1:98:A:LEU:CG	10	6.86
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	12	6.78
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	17	6.75
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	1	6.54
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	4	6.4
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	19	6.26
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	15	6.23
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	10	6.18
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	5	6.06
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	16	5.91
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	7	5.78
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	19	5.76
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	20	5.76
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	8	5.66
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	8	5.61
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	15	5.59
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	17	5.5
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	7	5.47
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	3	5.45
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	20	5.38
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	5	5.32
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	6	5.31
(1,228)	1:55:A:ARG:CA	1:55:A:ARG:CB	1:55:A:ARG:CG	1:55:A:ARG:CD	14	5.23
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	10	5.17
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	9	5.17
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	16	5.17
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	11	5.14
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	5	4.99
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	2	4.98
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	6	4.83
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	6	4.81
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	13	4.78
(1,128)	1:13:A:ASN:CA	1:13:A:ASN:CB	1:13:A:ASN:CG	1:13:A:ASN:OD1	20	4.78
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	14	4.72
(1,182)	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	1:35:A:SER:N	14	4.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	18	4.66
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	19	4.44
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	13	4.43
(1,304)	1:94:A:VAL:N	1:94:A:VAL:CA	1:94:A:VAL:CB	1:94:A:VAL:CG1	19	4.38
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	12	4.38
(1,309)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:CB	1:98:A:LEU:CG	5	4.35
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	20	4.31
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	14	4.31
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	1	4.25
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	5	4.24
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	3	4.07
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	13	4.05
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	2	4.01
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	3	3.95
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	1	3.91
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	11	3.85
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	12	3.85
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	15	3.74
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	7	3.71
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	12	3.67
(1,113)	1:6:A:ARG:N	1:6:A:ARG:CA	1:6:A:ARG:C	1:7:A:THR:N	2	3.54
(1,274)	1:75:A:GLN:CA	1:75:A:GLN:CB	1:75:A:GLN:CG	1:75:A:GLN:CD	6	3.53
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	20	3.51
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	3	3.45
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	12	3.41
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	15	3.38
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	11	3.33
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	7	3.27
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	17	3.05
(1,315)	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:CB	1:101:A:GLU:CG	15	3.01
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	14	2.95
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	8	2.93
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	19	2.93
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	7	2.91
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	15	2.89
(1,299)	1:88:A:ILE:N	1:88:A:ILE:CA	1:88:A:ILE:CB	1:88:A:ILE:CG1	10	2.83
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	4	2.82
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	17	2.82
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	10	2.8
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	12	2.78
(1,253)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:CB	1:64:A:ILE:CG1	3	2.76
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	13	2.71
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	1	2.64
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	10	2.63
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	7	2.63
(1,294)	1:83:A:ASN:CA	1:83:A:ASN:CB	1:83:A:ASN:CG	1:83:A:ASN:OD1	13	2.62
(1,58)	1:72:A:ILE:C	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:C	9	2.61
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	18	2.58
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	14	2.55
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	8	2.48
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	3	2.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,196)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:CB	1:43:A:ILE:CG1	9	2.44
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	15	2.39
(1,100)	1:97:A:GLU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	3	2.39
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	15	2.33
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	5	2.31
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	13	2.26
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	16	2.24
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	6	2.2
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	20	2.2
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	2	2.19
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	7	2.18
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	18	2.17
(1,33)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ASP:N	10	2.16
(1,331)	1:105:A:ARG:N	1:105:A:ARG:CA	1:105:A:ARG:C	1:106:A:ARG:N	10	2.11
(1,291)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:CB	1:81:A:GLU:CG	6	2.08
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	1	2.05
(1,7)	1:7:A:THR:C	1:8:A:VAL:N	1:8:A:VAL:CA	1:8:A:VAL:C	6	2.02
(1,275)	1:75:A:GLN:C	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	19	1.98
(1,253)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:CB	1:64:A:ILE:CG1	11	1.96
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	16	1.96
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	18	1.95
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1	1.94
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	2	1.92
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	17	1.9
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	14	1.85
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	18	1.84
(1,38)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	15	1.83
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	9	1.83
(1,210)	1:47:A:GLY:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	16	1.82
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	2	1.82
(1,309)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:CB	1:98:A:LEU:CG	15	1.81
(1,228)	1:55:A:ARG:CA	1:55:A:ARG:CB	1:55:A:ARG:CG	1:55:A:ARG:CD	17	1.8
(1,163)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:HIS:N	10	1.78
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	5	1.73
(1,213)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:PRO:N	20	1.7
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	4	1.7
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	17	1.69
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	15	1.66
(1,309)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:CB	1:98:A:LEU:CG	2	1.64
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	13	1.63
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	12	1.62
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	15	1.6
(1,97)	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1:97:A:GLU:N	18	1.59
(1,260)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:ASP:N	19	1.58
(1,212)	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	1:48:A:LEU:CD1	5	1.57
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	7	1.57
(1,33)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ASP:N	18	1.55
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	5	1.53
(1,5)	1:4:A:ILE:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	14	1.52
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	12	1.5
(1,331)	1:105:A:ARG:N	1:105:A:ARG:CA	1:105:A:ARG:C	1:106:A:ARG:N	6	1.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,49)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:THR:N	1	1.49
(1,266)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:CB	1:69:A:VAL:CG1	11	1.47
(1,163)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:HIS:N	12	1.47
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	4	1.45
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	8	1.44
(1,189)	1:39:A:LEU:CA	1:39:A:LEU:CB	1:39:A:LEU:CG	1:39:A:LEU:CD1	9	1.44
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	13	1.43
(1,61)	1:74:A:ALA:N	1:74:A:ALA:CA	1:74:A:ALA:C	1:75:A:GLN:N	20	1.43
(1,33)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ASP:N	12	1.43
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:SER:N	14	1.43
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	17	1.42
(1,45)	1:55:A:ARG:N	1:55:A:ARG:CA	1:55:A:ARG:C	1:56:A:LEU:N	9	1.41
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	18	1.37
(1,248)	1:62:A:HIS:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	16	1.36
(1,210)	1:47:A:GLY:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	2	1.32
(1,138)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:CB	1:17:A:ILE:CG1	14	1.29
(1,278)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:PHE:N	6	1.28
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	20	1.28
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	6	1.27
(1,204)	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	1:46:A:SER:N	3	1.26
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	5	1.26
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	4	1.26
(1,210)	1:47:A:GLY:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	12	1.25
(1,58)	1:72:A:ILE:C	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:C	2	1.25
(1,19)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	2	1.24
(1,198)	1:43:A:ILE:N	1:43:A:ILE:CA	1:43:A:ILE:C	1:44:A:ARG:N	11	1.23
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	6	1.23
(1,211)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:CB	1:48:A:LEU:CG	14	1.2
(1,103)	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1:101:A:GLU:N	15	1.2
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	4	1.2
(1,35)	1:42:A:ASP:N	1:42:A:ASP:CA	1:42:A:ASP:C	1:43:A:ILE:N	5	1.2
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:SER:N	2	1.2
(1,2)	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	1:3:A:ALA:N	7	1.19
(1,321)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LYS:N	13	1.17
(1,138)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:CB	1:17:A:ILE:CG1	9	1.17
(1,210)	1:47:A:GLY:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	9	1.16
(1,128)	1:13:A:ASN:CA	1:13:A:ASN:CB	1:13:A:ASN:CG	1:13:A:ASN:OD1	18	1.16
(1,57)	1:72:A:ILE:N	1:72:A:ILE:CA	1:72:A:ILE:C	1:73:A:LYS:N	7	1.16
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	18	1.13
(1,236)	1:58:A:THR:N	1:58:A:THR:CA	1:58:A:THR:C	1:59:A:ALA:N	3	1.11
(1,97)	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1:97:A:GLU:N	11	1.11
(1,38)	1:51:A:TYR:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	3	1.11
(1,213)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:PRO:N	13	1.09
(1,67)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:LEU:N	19	1.08
(1,17)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:THR:N	7	1.08
(1,138)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:CB	1:17:A:ILE:CG1	17	1.07
(1,63)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	1	1.07
(1,35)	1:42:A:ASP:N	1:42:A:ASP:CA	1:42:A:ASP:C	1:43:A:ILE:N	13	1.07
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	5	1.07
(1,24)	1:36:A:ALA:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	4	1.07
(1,62)	1:74:A:ALA:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	11	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	1:40:A:ARG:N	17	1.06
(1,46)	1:55:A:ARG:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	5	1.02
(1,51)	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	1:70:A:ILE:N	9	1.01