



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:30 AM UTC

PDB ID : 2K5G / pdb_00002k5g
BMRB ID : 15835
Title : Solution NMR structure of protein encoded by gene BPP1335 from Bordetella parapertussis: Northeast Structural Genomics Target BpR195
Authors : Singarapu, K.; Eletsky, A.; Sathyamoorthy, B.; Sukumaran, D.; Wang, D.; Jiang, M.; Ciccocanti, C.; Xiao, R.; Liu, J.; Baran, M.C.; Swapna, G.; Acton, T.B.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-06-27

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

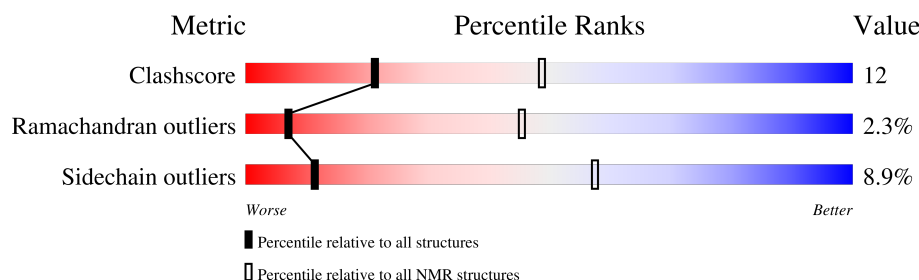
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	191	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:19-A:64, A:75-A:107, A:111-A:180 (149)	1.26	6

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2958 atoms, of which 1460 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			2958	947	1460	283	265	3	

There are 8 discrepancies between the modelled and reference sequences:

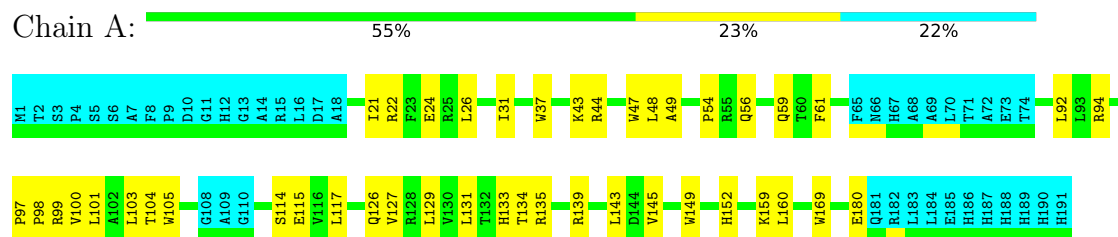
Chain	Residue	Modelled	Actual	Comment	Reference
A	184	LEU	-	expression tag	UNP Q7WAN9
A	185	GLU	-	expression tag	UNP Q7WAN9
A	186	HIS	-	expression tag	UNP Q7WAN9
A	187	HIS	-	expression tag	UNP Q7WAN9
A	188	HIS	-	expression tag	UNP Q7WAN9
A	189	HIS	-	expression tag	UNP Q7WAN9
A	190	HIS	-	expression tag	UNP Q7WAN9
A	191	HIS	-	expression tag	UNP Q7WAN9

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: uncharacterized protein

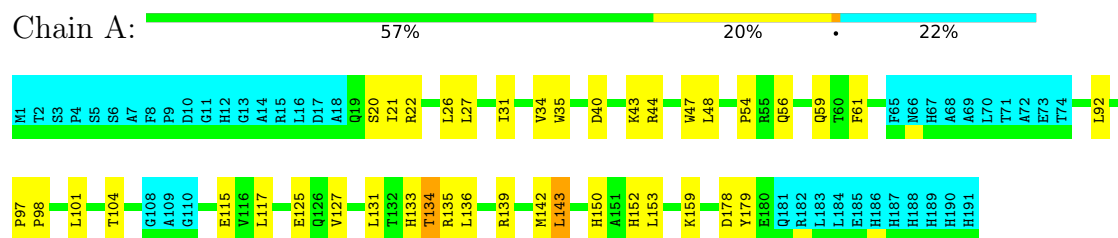


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

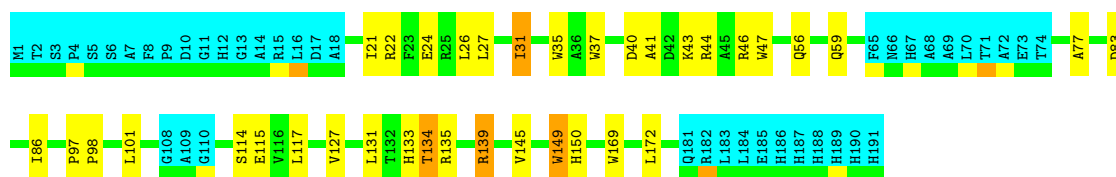
- Molecule 1: uncharacterized protein



4.2.2 Score per residue for model 2

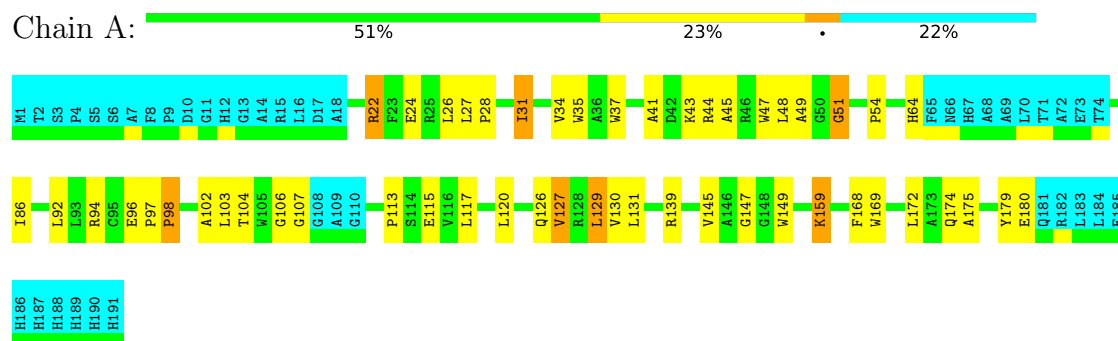
- Molecule 1: uncharacterized protein





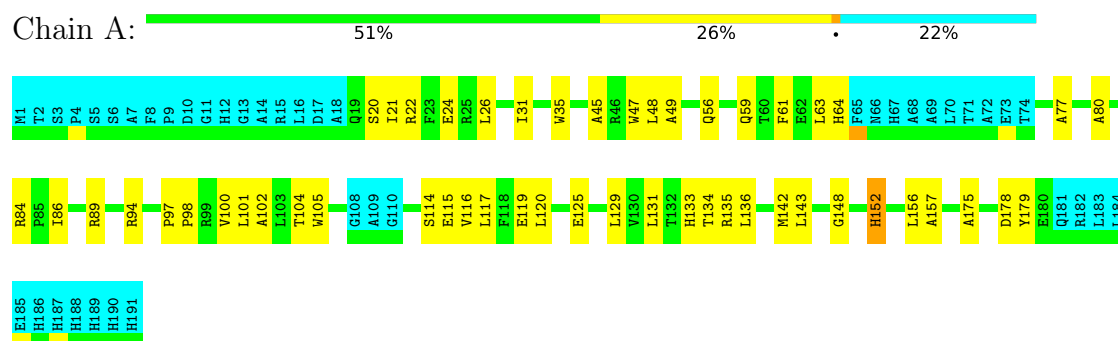
4.2.3 Score per residue for model 3

- Molecule 1: uncharacterized protein



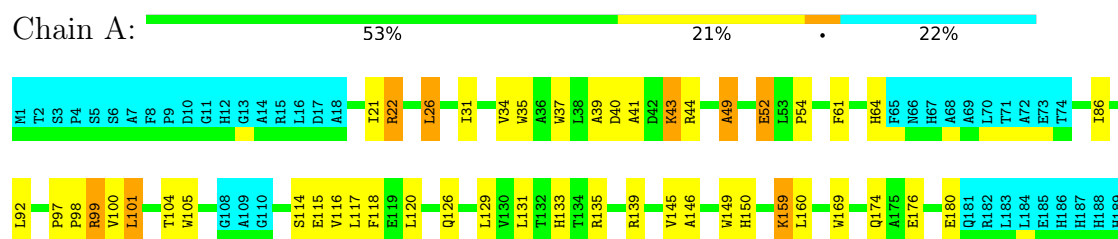
4.2.4 Score per residue for model 4

- Molecule 1: uncharacterized protein



4.2.5 Score per residue for model 5

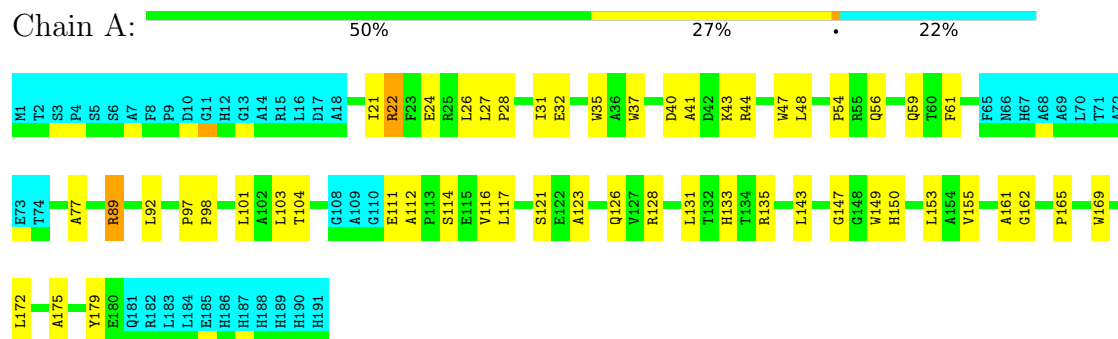
- Molecule 1: uncharacterized protein



H190
H191

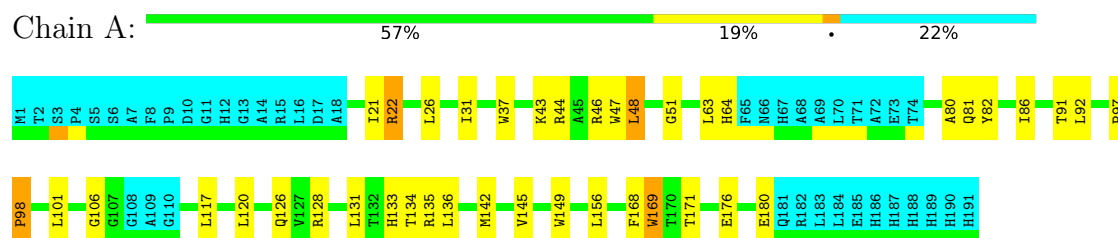
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: uncharacterized protein



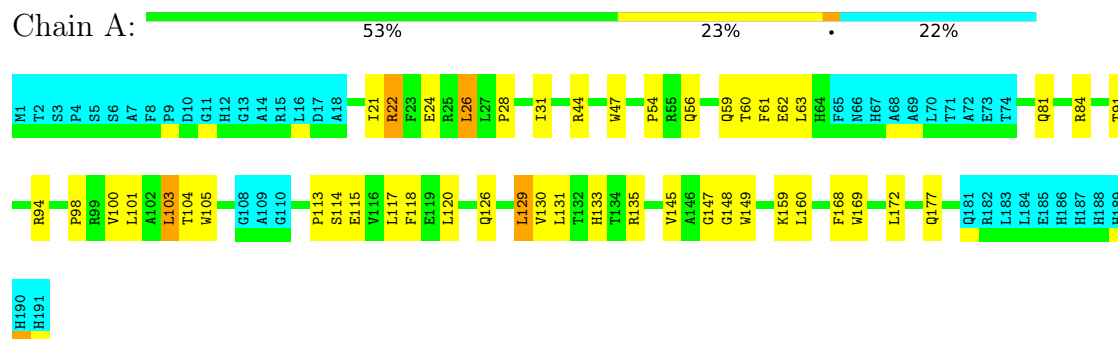
4.2.7 Score per residue for model 7

- Molecule 1: uncharacterized protein



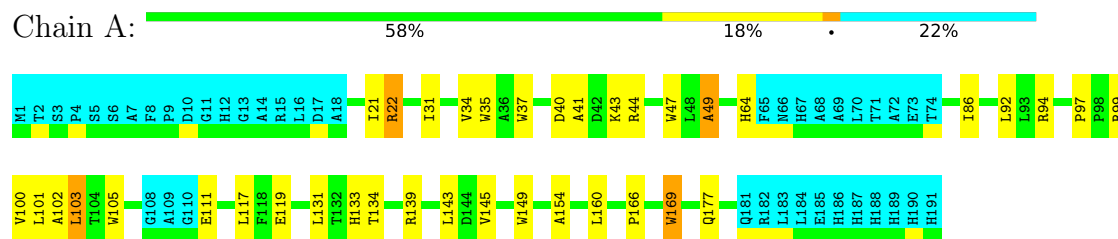
4.2.8 Score per residue for model 8

- Molecule 1: uncharacterized protein



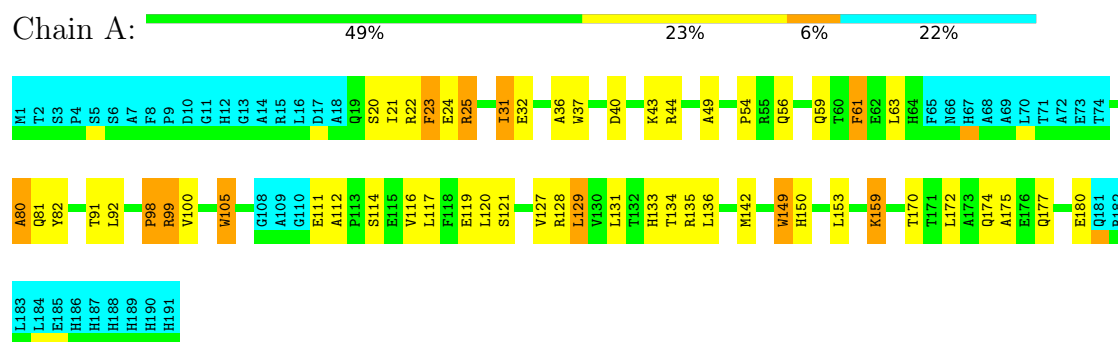
4.2.9 Score per residue for model 9

- Molecule 1: uncharacterized protein



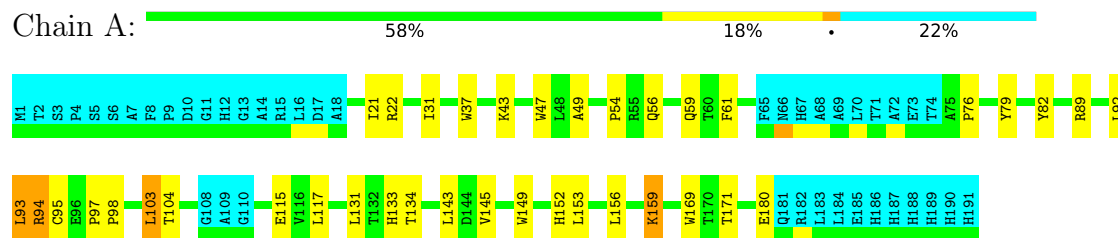
4.2.10 Score per residue for model 10

- Molecule 1: uncharacterized protein



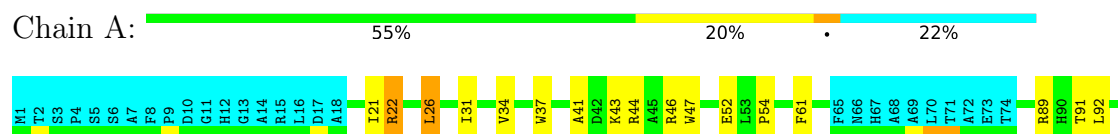
4.2.11 Score per residue for model 11

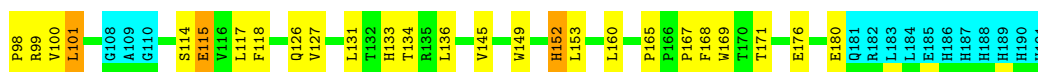
- Molecule 1: uncharacterized protein



4.2.12 Score per residue for model 12

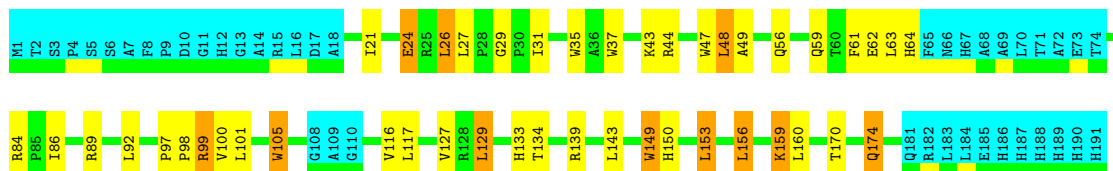
- Molecule 1: uncharacterized protein





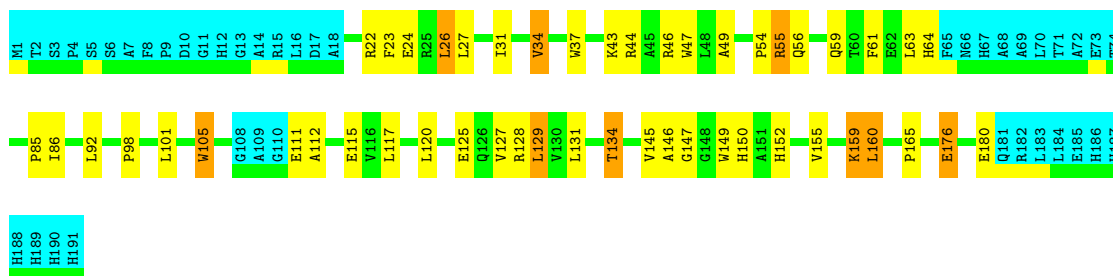
4.2.13 Score per residue for model 13

- Molecule 1: uncharacterized protein



4.2.14 Score per residue for model 14

- Molecule 1: uncharacterized protein



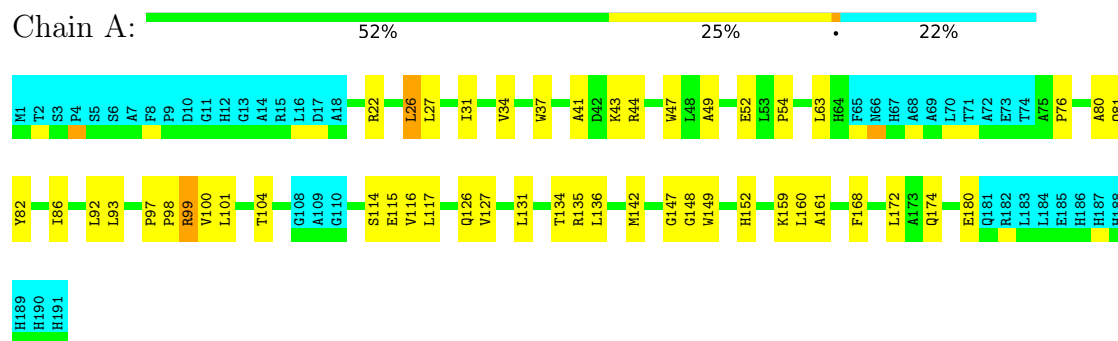
4.2.15 Score per residue for model 15

- Molecule 1: uncharacterized protein



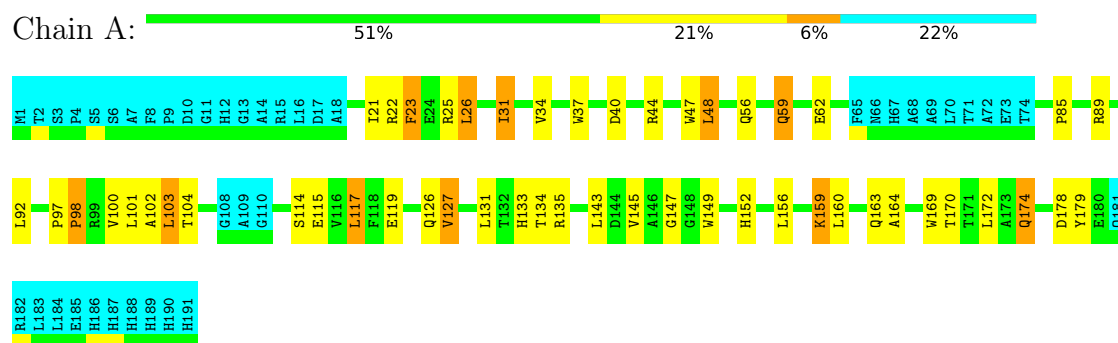
4.2.16 Score per residue for model 16

- Molecule 1: uncharacterized protein



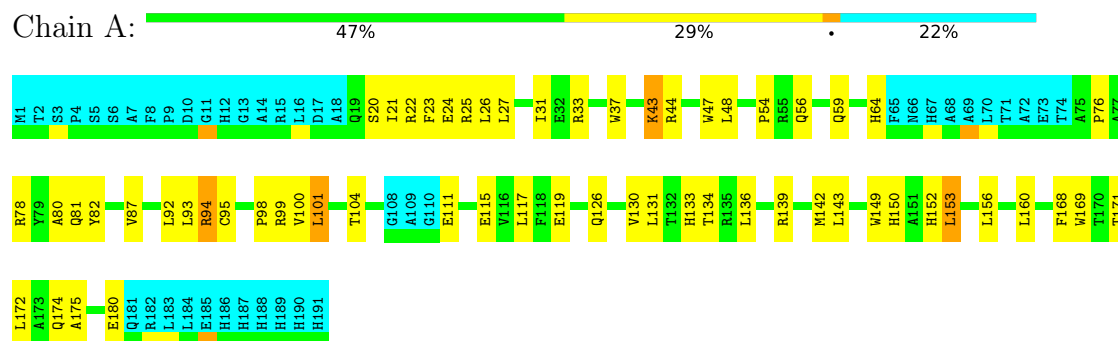
4.2.17 Score per residue for model 17

- Molecule 1: uncharacterized protein



4.2.18 Score per residue for model 18

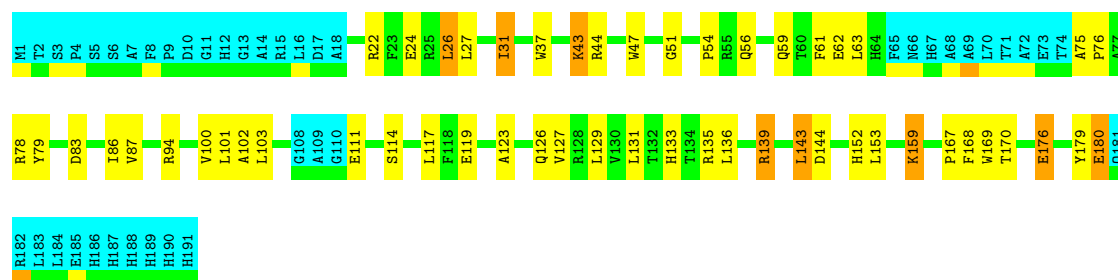
- Molecule 1: uncharacterized protein



4.2.19 Score per residue for model 19

- Molecule 1: uncharacterized protein





4.2.20 Score per residue for model 20

- Molecule 1: uncharacterized protein

Chain A: 49% 26% 22%



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: *structures with the lowest energy*.

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

Software name	Classification	Version
AutoStructure	structure solution	
CNS	refinement	
CYANA	structure solution	
MOLMOL	structure solution	
PSVS	geometry optimization	

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	2137
Number of shifts mapped to atoms	2137
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1178	1166	1161	28±6
All	All	23560	23320	23220	551

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:TRP:HB3	1:A:43:LYS:HD3	0.88	1.43	14	3
1:A:44:ARG:HB3	1:A:47:TRP:HD1	0.88	1.26	15	1
1:A:20:SER:HA	1:A:136:LEU:HD12	0.86	1.45	1	4
1:A:21:ILE:HB	1:A:133:HIS:HB3	0.86	1.43	5	15
1:A:114:SER:HA	1:A:135:ARG:HB3	0.86	1.43	4	4
1:A:37:TRP:CE3	1:A:43:LYS:HE3	0.84	2.07	20	1
1:A:100:VAL:HG12	1:A:119:GLU:HA	0.83	1.51	10	6
1:A:41:ALA:HA	1:A:44:ARG:HG2	0.81	1.52	12	4
1:A:44:ARG:HB3	1:A:47:TRP:CD1	0.80	2.12	15	2
1:A:44:ARG:HD3	1:A:47:TRP:CD1	0.76	2.15	19	1
1:A:111:GLU:HG3	1:A:112:ALA:H	0.76	1.40	10	2
1:A:114:SER:HA	1:A:135:ARG:HB2	0.74	1.57	2	5
1:A:136:LEU:HD13	1:A:142:MET:HG2	0.74	1.58	18	6
1:A:41:ALA:HA	1:A:51:GLY:HA3	0.73	1.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LYS:HE3	1:A:159:LYS:HA	0.73	1.59	13	4
1:A:45:ALA:HA	1:A:49:ALA:HA	0.73	1.58	3	2
1:A:49:ALA:HB1	1:A:64:HIS:HB2	0.73	1.61	14	2
1:A:61:PHE:HE2	1:A:92:LEU:HB3	0.72	1.44	13	1
1:A:34:VAL:HG21	1:A:127:VAL:HG21	0.72	1.60	3	2
1:A:147:GLY:HA2	1:A:172:LEU:HD11	0.72	1.62	6	3
1:A:37:TRP:HE1	1:A:160:LEU:HD11	0.69	1.48	18	3
1:A:37:TRP:CD1	1:A:160:LEU:HD21	0.69	2.22	14	3
1:A:26:LEU:HD11	1:A:126:GLN:HB3	0.68	1.66	6	9
1:A:139:ARG:HD2	1:A:139:ARG:H	0.67	1.48	13	3
1:A:94:ARG:H	1:A:102:ALA:HB3	0.67	1.50	20	4
1:A:76:PRO:HD2	1:A:79:TYR:HD2	0.67	1.50	19	2
1:A:56:GLN:HB2	1:A:59:GLN:HG3	0.67	1.66	20	6
1:A:54:PRO:HD3	1:A:61:PHE:HB3	0.67	1.66	11	5
1:A:154:ALA:HB1	1:A:166:PRO:HG2	0.66	1.65	9	1
1:A:37:TRP:HA	1:A:43:LYS:HD2	0.66	1.64	9	4
1:A:152:HIS:O	1:A:156:LEU:HG	0.66	1.91	18	2
1:A:159:LYS:HE2	1:A:159:LYS:HA	0.65	1.66	16	4
1:A:147:GLY:HA3	1:A:176:GLU:HG2	0.65	1.66	20	2
1:A:37:TRP:HB2	1:A:47:TRP:HE1	0.65	1.51	14	1
1:A:99:ARG:HG3	1:A:100:VAL:HG23	0.65	1.69	13	4
1:A:44:ARG:HA	1:A:47:TRP:NE1	0.64	2.08	13	9
1:A:21:ILE:HB	1:A:133:HIS:CB	0.63	2.23	1	2
1:A:34:VAL:HG21	1:A:127:VAL:HG11	0.63	1.70	14	4
1:A:99:ARG:HG3	1:A:100:VAL:HG13	0.62	1.71	18	2
1:A:23:PHE:HE1	1:A:131:LEU:HD13	0.62	1.53	10	1
1:A:22:ARG:HA	1:A:131:LEU:O	0.61	1.94	8	18
1:A:131:LEU:HD13	1:A:153:LEU:HD21	0.61	1.72	12	2
1:A:61:PHE:CE2	1:A:92:LEU:HB3	0.61	2.30	13	1
1:A:41:ALA:CA	1:A:51:GLY:HA3	0.61	2.26	3	1
1:A:104:THR:HA	1:A:115:GLU:HA	0.61	1.73	15	11
1:A:92:LEU:HA	1:A:103:LEU:HA	0.61	1.73	9	3
1:A:44:ARG:NH1	1:A:52:GLU:HA	0.61	2.11	5	1
1:A:44:ARG:HD3	1:A:47:TRP:HD1	0.61	1.53	19	1
1:A:176:GLU:O	1:A:180:GLU:HB2	0.60	1.97	12	5
1:A:54:PRO:HD2	1:A:92:LEU:HD22	0.60	1.73	16	1
1:A:44:ARG:HA	1:A:47:TRP:CD1	0.60	2.32	20	13
1:A:64:HIS:HA	1:A:86:ILE:O	0.59	1.97	14	3
1:A:92:LEU:H	1:A:92:LEU:HD23	0.59	1.57	14	4
1:A:34:VAL:CG2	1:A:127:VAL:HG11	0.59	2.27	14	1
1:A:105:TRP:NE1	1:A:145:VAL:HG12	0.59	2.12	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:PRO:HD2	1:A:92:LEU:HD13	0.59	1.73	6	1
1:A:43:LYS:HD3	1:A:44:ARG:CD	0.59	2.27	19	1
1:A:45:ALA:HA	1:A:49:ALA:CA	0.59	2.27	3	2
1:A:139:ARG:HA	1:A:142:MET:SD	0.59	2.36	1	1
1:A:37:TRP:O	1:A:44:ARG:HG3	0.59	1.98	19	1
1:A:23:PHE:CE1	1:A:131:LEU:HD13	0.59	2.32	10	1
1:A:37:TRP:NE1	1:A:160:LEU:HD11	0.59	2.12	17	2
1:A:123:ALA:HB3	1:A:126:GLN:HG3	0.59	1.74	19	1
1:A:31:ILE:HA	1:A:127:VAL:HG11	0.58	1.75	17	3
1:A:150:HIS:CE1	1:A:175:ALA:HB3	0.57	2.33	10	1
1:A:44:ARG:HD3	1:A:51:GLY:HA2	0.57	1.76	3	1
1:A:111:GLU:HG3	1:A:112:ALA:N	0.57	2.14	15	4
1:A:21:ILE:HG22	1:A:133:HIS:HB3	0.57	1.76	17	1
1:A:93:LEU:HG	1:A:94:ARG:H	0.57	1.58	18	1
1:A:54:PRO:HG3	1:A:61:PHE:HB3	0.57	1.76	14	6
1:A:94:ARG:HB3	1:A:102:ALA:HB3	0.57	1.76	19	2
1:A:41:ALA:HA	1:A:44:ARG:CG	0.57	2.29	12	3
1:A:34:VAL:HA	1:A:160:LEU:HD21	0.57	1.77	5	5
1:A:39:ALA:HA	1:A:44:ARG:NH2	0.57	2.15	5	1
1:A:37:TRP:CE3	1:A:43:LYS:HD2	0.57	2.34	16	2
1:A:37:TRP:CE3	1:A:43:LYS:HE2	0.56	2.34	9	2
1:A:24:GLU:HG3	1:A:130:VAL:HG23	0.56	1.77	18	1
1:A:37:TRP:HB3	1:A:43:LYS:CD	0.56	2.30	18	1
1:A:115:GLU:HG3	1:A:134:THR:OG1	0.56	2.01	1	2
1:A:41:ALA:HA	1:A:44:ARG:HB3	0.56	1.77	6	2
1:A:63:LEU:O	1:A:87:VAL:HA	0.56	2.01	19	2
1:A:145:VAL:HB	1:A:149:TRP:CD1	0.56	2.34	3	1
1:A:155:VAL:HG13	1:A:165:PRO:HB3	0.56	1.76	6	2
1:A:37:TRP:CD1	1:A:44:ARG:HH11	0.55	2.19	19	1
1:A:78:ARG:NH2	1:A:144:ASP:HA	0.55	2.16	19	1
1:A:44:ARG:HA	1:A:44:ARG:HE	0.55	1.61	19	1
1:A:143:LEU:HG	1:A:179:TYR:HB3	0.55	1.77	1	2
1:A:54:PRO:HG2	1:A:92:LEU:HD22	0.55	1.79	6	3
1:A:47:TRP:CE3	1:A:48:LEU:HB2	0.55	2.37	17	5
1:A:120:LEU:HD21	1:A:129:LEU:HD12	0.55	1.78	10	4
1:A:49:ALA:HB1	1:A:64:HIS:O	0.55	2.01	9	2
1:A:150:HIS:NE2	1:A:175:ALA:HB3	0.55	2.16	18	2
1:A:105:TRP:CD1	1:A:145:VAL:HG12	0.55	2.36	9	2
1:A:37:TRP:HB2	1:A:47:TRP:NE1	0.55	2.16	14	1
1:A:54:PRO:HD2	1:A:92:LEU:HD11	0.54	1.79	12	1
1:A:34:VAL:HG21	1:A:127:VAL:CG1	0.54	2.33	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ARG:HG3	1:A:49:ALA:O	0.54	2.02	16	1
1:A:169:TRP:HA	1:A:169:TRP:CE3	0.54	2.38	2	1
1:A:146:ALA:HA	1:A:150:HIS:ND1	0.54	2.17	14	1
1:A:145:VAL:HB	1:A:149:TRP:HD1	0.54	1.63	3	1
1:A:37:TRP:CE3	1:A:43:LYS:CE	0.54	2.88	20	1
1:A:41:ALA:HB2	1:A:52:GLU:HG2	0.53	1.80	5	1
1:A:75:ALA:HB1	1:A:79:TYR:HB2	0.53	1.78	19	1
1:A:23:PHE:CD1	1:A:131:LEU:HB2	0.53	2.38	17	1
1:A:56:GLN:HB2	1:A:59:GLN:CG	0.53	2.34	20	2
1:A:147:GLY:HA2	1:A:172:LEU:HG	0.53	1.80	8	2
1:A:94:ARG:HD3	1:A:96:GLU:OE1	0.53	2.03	3	1
1:A:37:TRP:O	1:A:44:ARG:HB3	0.53	2.03	14	1
1:A:77:ALA:HA	1:A:80:ALA:HB3	0.52	1.80	20	1
1:A:76:PRO:HG2	1:A:78:ARG:HG2	0.52	1.81	18	1
1:A:37:TRP:CZ2	1:A:156:LEU:HD11	0.52	2.39	13	1
1:A:35:TRP:CZ2	1:A:97:PRO:HB3	0.52	2.39	2	10
1:A:133:HIS:CE1	1:A:145:VAL:HG11	0.52	2.40	2	3
1:A:105:TRP:HB2	1:A:116:VAL:HG23	0.52	1.80	15	3
1:A:48:LEU:O	1:A:48:LEU:HD13	0.52	2.05	3	2
1:A:115:GLU:HG2	1:A:135:ARG:HB2	0.52	1.82	1	1
1:A:43:LYS:HD3	1:A:44:ARG:CG	0.52	2.35	19	1
1:A:47:TRP:CE3	1:A:156:LEU:HB3	0.51	2.40	11	1
1:A:55:ARG:NE	1:A:55:ARG:HA	0.51	2.21	14	1
1:A:40:ASP:O	1:A:44:ARG:HB2	0.51	2.06	10	3
1:A:103:LEU:N	1:A:103:LEU:HD13	0.51	2.21	17	5
1:A:145:VAL:HB	1:A:149:TRP:HB3	0.50	1.81	14	2
1:A:47:TRP:HZ3	1:A:152:HIS:HD2	0.50	1.48	11	1
1:A:149:TRP:CE3	1:A:152:HIS:HE1	0.50	2.24	16	1
1:A:149:TRP:HE3	1:A:152:HIS:HE2	0.50	1.48	18	1
1:A:93:LEU:HD12	1:A:94:ARG:HG3	0.50	1.83	11	1
1:A:40:ASP:OD2	1:A:43:LYS:HG2	0.50	2.07	9	5
1:A:149:TRP:HA	1:A:149:TRP:CE3	0.50	2.41	10	2
1:A:134:THR:O	1:A:135:ARG:HB2	0.50	2.07	7	1
1:A:76:PRO:HD2	1:A:79:TYR:CD2	0.50	2.38	19	2
1:A:47:TRP:CZ3	1:A:156:LEU:HG	0.49	2.42	15	1
1:A:25:ARG:HA	1:A:25:ARG:HE	0.49	1.67	10	1
1:A:133:HIS:CE1	1:A:136:LEU:HD21	0.49	2.42	15	3
1:A:63:LEU:HG	1:A:64:HIS:H	0.49	1.66	14	1
1:A:43:LYS:HD3	1:A:44:ARG:HG2	0.49	1.84	19	1
1:A:113:PRO:O	1:A:135:ARG:HD3	0.49	2.07	8	1
1:A:167:PRO:HB2	1:A:170:THR:HB	0.49	1.85	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:TRP:HE1	1:A:145:VAL:HG12	0.49	1.67	5	1
1:A:32:GLU:HG2	1:A:98:PRO:HG2	0.49	1.82	10	1
1:A:139:ARG:O	1:A:142:MET:HG2	0.48	2.09	1	1
1:A:43:LYS:CD	1:A:44:ARG:HG2	0.48	2.38	19	1
1:A:123:ALA:HB3	1:A:126:GLN:HB2	0.48	1.85	6	1
1:A:80:ALA:O	1:A:82:TYR:N	0.48	2.47	10	3
1:A:25:ARG:HA	1:A:25:ARG:NE	0.48	2.24	10	1
1:A:44:ARG:CB	1:A:47:TRP:HD1	0.48	2.12	15	1
1:A:26:LEU:HD11	1:A:126:GLN:HB2	0.48	1.83	8	1
1:A:27:LEU:HD22	1:A:160:LEU:HD12	0.48	1.84	13	1
1:A:105:TRP:C	1:A:105:TRP:CD1	0.48	2.92	10	1
1:A:37:TRP:CG	1:A:43:LYS:HD3	0.48	2.44	11	1
1:A:148:GLY:O	1:A:150:HIS:N	0.48	2.46	20	1
1:A:116:VAL:HG21	1:A:149:TRP:CZ2	0.48	2.44	16	3
1:A:150:HIS:NE2	1:A:172:LEU:HD12	0.48	2.23	2	1
1:A:114:SER:HA	1:A:135:ARG:CB	0.48	2.39	10	3
1:A:37:TRP:CB	1:A:43:LYS:HD3	0.48	2.33	13	1
1:A:54:PRO:HG2	1:A:92:LEU:HB2	0.48	1.84	18	1
1:A:35:TRP:HA	1:A:38:LEU:HD12	0.48	1.85	20	1
1:A:37:TRP:CD1	1:A:43:LYS:HD2	0.47	2.44	3	1
1:A:102:ALA:HB2	1:A:117:LEU:HD22	0.47	1.86	17	1
1:A:31:ILE:HA	1:A:127:VAL:CG2	0.47	2.39	19	2
1:A:43:LYS:HD3	1:A:44:ARG:HD2	0.47	1.86	19	1
1:A:24:GLU:HA	1:A:129:LEU:O	0.47	2.10	13	3
1:A:159:LYS:HA	1:A:159:LYS:CE	0.47	2.40	5	2
1:A:25:ARG:HD2	1:A:153:LEU:HB3	0.47	1.86	10	1
1:A:131:LEU:HD22	1:A:153:LEU:HD21	0.47	1.87	11	1
1:A:148:GLY:HA2	1:A:168:PHE:CZ	0.46	2.44	8	1
1:A:62:GLU:HA	1:A:89:ARG:HA	0.46	1.87	17	2
1:A:155:VAL:HG13	1:A:165:PRO:CB	0.46	2.40	14	1
1:A:101:LEU:HG	1:A:118:PHE:HB2	0.46	1.87	15	3
1:A:105:TRP:HA	1:A:105:TRP:CE3	0.46	2.45	13	2
1:A:46:ARG:O	1:A:46:ARG:HD3	0.46	2.10	2	1
1:A:54:PRO:CD	1:A:61:PHE:HB3	0.46	2.40	15	1
1:A:23:PHE:HD2	1:A:131:LEU:HD23	0.46	1.69	18	1
1:A:133:HIS:HE1	1:A:145:VAL:HG11	0.46	1.71	2	2
1:A:145:VAL:O	1:A:149:TRP:HB3	0.46	2.10	11	6
1:A:44:ARG:HE	1:A:44:ARG:CA	0.46	2.23	19	1
1:A:106:GLY:C	1:A:113:PRO:HB3	0.46	2.36	3	1
1:A:24:GLU:HG2	1:A:130:VAL:HG22	0.46	1.87	8	1
1:A:40:ASP:HB3	1:A:43:LYS:HE2	0.46	1.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLY:HA3	1:A:63:LEU:HD23	0.46	1.88	7	1
1:A:80:ALA:O	1:A:81:GLN:HG2	0.46	2.10	18	1
1:A:150:HIS:O	1:A:153:LEU:HB2	0.46	2.10	13	2
1:A:98:PRO:O	1:A:99:ARG:HD2	0.46	2.11	10	1
1:A:61:PHE:O	1:A:89:ARG:HA	0.45	2.10	12	4
1:A:26:LEU:HD13	1:A:27:LEU:N	0.45	2.26	3	9
1:A:43:LYS:HB2	1:A:43:LYS:NZ	0.45	2.26	5	1
1:A:134:THR:HG22	1:A:135:ARG:H	0.45	1.71	10	1
1:A:44:ARG:HH12	1:A:52:GLU:HA	0.45	1.71	5	1
1:A:84:ARG:O	1:A:86:ILE:HG13	0.45	2.11	13	1
1:A:121:SER:HB2	1:A:128:ARG:CG	0.45	2.42	10	1
1:A:114:SER:HB3	1:A:134:THR:O	0.45	2.12	12	1
1:A:62:GLU:HG2	1:A:89:ARG:HB3	0.45	1.89	13	1
1:A:23:PHE:HD1	1:A:131:LEU:CB	0.45	2.25	17	1
1:A:81:GLN:HG3	1:A:84:ARG:CZ	0.45	2.42	8	1
1:A:120:LEU:CD2	1:A:129:LEU:HB2	0.45	2.42	15	3
1:A:95:CYS:HA	1:A:101:LEU:HA	0.45	1.89	18	1
1:A:23:PHE:CD1	1:A:131:LEU:CB	0.44	3.00	17	1
1:A:43:LYS:HG3	1:A:44:ARG:HG2	0.44	1.89	19	1
1:A:107:GLY:HA2	1:A:113:PRO:HG3	0.44	1.89	20	1
1:A:56:GLN:HB2	1:A:59:GLN:CD	0.44	2.38	19	7
1:A:37:TRP:CD1	1:A:43:LYS:HD3	0.44	2.48	6	1
1:A:105:TRP:O	1:A:114:SER:HB2	0.44	2.13	8	1
1:A:177:GLN:HA	1:A:177:GLN:OE1	0.44	2.13	9	1
1:A:37:TRP:HE3	1:A:43:LYS:HE3	0.44	1.65	20	1
1:A:63:LEU:C	1:A:63:LEU:HD12	0.44	2.38	4	1
1:A:95:CYS:O	1:A:97:PRO:HD3	0.44	2.13	11	1
1:A:44:ARG:HA	1:A:44:ARG:NE	0.44	2.27	19	1
1:A:20:SER:HB3	1:A:133:HIS:O	0.44	2.12	1	2
1:A:143:LEU:HD21	1:A:179:TYR:HB2	0.44	1.88	4	2
1:A:40:ASP:OD2	1:A:43:LYS:HB2	0.44	2.13	5	1
1:A:24:GLU:HA	1:A:130:VAL:HA	0.43	1.90	3	1
1:A:120:LEU:HA	1:A:128:ARG:O	0.43	2.13	7	1
1:A:100:VAL:HG23	1:A:118:PHE:O	0.43	2.13	8	1
1:A:28:PRO:HD2	1:A:160:LEU:HB3	0.43	1.90	8	1
1:A:150:HIS:HE1	1:A:172:LEU:HA	0.43	1.74	10	1
1:A:80:ALA:C	1:A:82:TYR:H	0.43	2.22	18	1
1:A:116:VAL:HG11	1:A:149:TRP:CH2	0.43	2.48	6	1
1:A:34:VAL:HA	1:A:37:TRP:NE1	0.43	2.28	14	1
1:A:44:ARG:HB3	1:A:47:TRP:NE1	0.43	2.29	19	1
1:A:131:LEU:HD12	1:A:153:LEU:HD21	0.43	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ALA:O	1:A:84:ARG:HG2	0.43	2.14	4	1
1:A:34:VAL:HG21	1:A:127:VAL:CG2	0.43	2.43	17	1
1:A:51:GLY:HA2	1:A:62:GLU:O	0.43	2.13	19	1
1:A:116:VAL:HG11	1:A:149:TRP:CZ2	0.43	2.49	10	2
1:A:41:ALA:CA	1:A:44:ARG:HG2	0.43	2.35	12	1
1:A:97:PRO:HA	1:A:98:PRO:HA	0.42	1.69	16	4
1:A:89:ARG:C	1:A:89:ARG:HD2	0.42	2.38	6	1
1:A:37:TRP:HA	1:A:43:LYS:CD	0.42	2.41	9	2
1:A:149:TRP:O	1:A:152:HIS:HD2	0.42	1.97	12	1
1:A:146:ALA:HA	1:A:150:HIS:CE1	0.42	2.49	5	1
1:A:170:THR:O	1:A:174:GLN:HB2	0.42	2.14	17	2
1:A:61:PHE:CE2	1:A:63:LEU:HG	0.42	2.50	15	1
1:A:115:GLU:HG2	1:A:134:THR:HB	0.42	1.90	2	1
1:A:34:VAL:HA	1:A:37:TRP:HE1	0.42	1.73	14	1
1:A:129:LEU:HD23	1:A:129:LEU:C	0.42	2.39	3	1
1:A:63:LEU:HG	1:A:64:HIS:N	0.42	2.29	14	1
1:A:153:LEU:HD13	1:A:156:LEU:HD12	0.42	1.90	18	1
1:A:156:LEU:HD12	1:A:157:ALA:N	0.42	2.29	4	1
1:A:59:GLN:O	1:A:92:LEU:HD23	0.42	2.13	17	1
1:A:131:LEU:HD11	1:A:149:TRP:HE1	0.42	1.75	8	1
1:A:154:ALA:HB1	1:A:166:PRO:CG	0.42	2.41	9	1
1:A:46:ARG:HA	1:A:46:ARG:HE	0.42	1.75	14	1
1:A:37:TRP:CH2	1:A:156:LEU:HD13	0.42	2.50	18	1
1:A:43:LYS:C	1:A:44:ARG:HE	0.42	2.23	19	1
1:A:44:ARG:HG3	1:A:47:TRP:CZ2	0.42	2.50	1	1
1:A:37:TRP:CZ3	1:A:43:LYS:HE2	0.42	2.50	9	2
1:A:104:THR:HB	1:A:114:SER:O	0.42	2.15	5	1
1:A:76:PRO:HD3	1:A:169:TRP:HZ2	0.42	1.73	18	1
1:A:168:PHE:HA	1:A:171:THR:HG22	0.42	1.92	18	1
1:A:169:TRP:HA	1:A:169:TRP:HE3	0.41	1.74	2	1
1:A:56:GLN:HB3	1:A:59:GLN:NE2	0.41	2.30	17	1
1:A:91:THR:HG22	1:A:92:LEU:O	0.41	2.15	10	1
1:A:37:TRP:CE3	1:A:43:LYS:CD	0.41	3.03	16	1
1:A:43:LYS:HB2	1:A:43:LYS:HZ3	0.41	1.75	5	1
1:A:37:TRP:CD2	1:A:43:LYS:HD2	0.41	2.51	7	1
1:A:103:LEU:HD22	1:A:103:LEU:C	0.41	2.41	9	1
1:A:115:GLU:O	1:A:133:HIS:HA	0.41	2.15	12	1
1:A:20:SER:CA	1:A:136:LEU:HD12	0.41	2.32	1	1
1:A:36:ALA:HB3	1:A:37:TRP:CE3	0.41	2.50	20	2
1:A:93:LEU:CD1	1:A:94:ARG:HG3	0.41	2.45	11	1
1:A:49:ALA:HB3	1:A:63:LEU:HD12	0.41	1.92	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLY:O	1:A:127:VAL:HG23	0.41	2.16	13	1
1:A:47:TRP:HZ3	1:A:152:HIS:HD1	0.41	1.57	4	1
1:A:175:ALA:O	1:A:178:ASP:HB2	0.41	2.16	4	1
1:A:22:ARG:N	1:A:22:ARG:HD3	0.41	2.31	15	2
1:A:54:PRO:HD2	1:A:92:LEU:CD1	0.41	2.45	12	1
1:A:27:LEU:HB2	1:A:127:VAL:HG13	0.40	1.92	1	1
1:A:76:PRO:HD3	1:A:169:TRP:CZ2	0.40	2.51	18	1
1:A:31:ILE:HA	1:A:127:VAL:HG22	0.40	1.92	19	1
1:A:175:ALA:O	1:A:179:TYR:HD1	0.40	1.99	3	2
1:A:121:SER:HB2	1:A:128:ARG:HG2	0.40	1.93	10	1
1:A:34:VAL:CG2	1:A:127:VAL:HG21	0.40	2.47	17	1
1:A:121:SER:HB2	1:A:128:ARG:HB2	0.40	1.93	6	1
1:A:23:PHE:CE1	1:A:131:LEU:HB2	0.40	2.51	17	1
1:A:37:TRP:NE1	1:A:160:LEU:HD21	0.40	2.31	17	1
1:A:48:LEU:O	1:A:49:ALA:HB3	0.40	2.17	4	1
1:A:64:HIS:CD2	1:A:87:VAL:HG22	0.40	2.51	18	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	149/191 (78%)	131±3 (88±2%)	14±3 (10±2%)	3±1 (2±1%)	7	45
All	All	2980/3820 (78%)	2623 (88%)	289 (10%)	68 (2%)	7	45

All 16 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	31	ILE	20
1	A	98	PRO	16
1	A	99	ARG	5
1	A	125	GLU	3
1	A	77	ALA	3
1	A	49	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	A	81	GLN	3
1	A	169	TRP	3
1	A	51	GLY	2
1	A	107	GLY	2
1	A	148	GLY	2
1	A	149	TRP	2
1	A	106	GLY	1
1	A	80	ALA	1
1	A	76	PRO	1
1	A	94	ARG	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	115/146 (79%)	105±2 (91±2%)	10±2 (9±2%)	11	57
All	All	2300/2920 (79%)	2095 (91%)	205 (9%)	11	57

All 52 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	117	LEU	20
1	A	101	LEU	17
1	A	26	LEU	12
1	A	134	THR	12
1	A	159	LYS	9
1	A	180	GLU	9
1	A	22	ARG	8
1	A	143	LEU	7
1	A	103	LEU	7
1	A	169	TRP	7
1	A	174	GLN	7
1	A	48	LEU	6
1	A	152	HIS	6
1	A	24	GLU	5
1	A	129	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	52	GLU	5
1	A	111	GLU	4
1	A	139	ARG	3
1	A	43	LYS	3
1	A	176	GLU	3
1	A	91	THR	3
1	A	156	LEU	3
1	A	171	THR	3
1	A	105	TRP	3
1	A	149	TRP	2
1	A	127	VAL	2
1	A	62	GLU	2
1	A	63	LEU	2
1	A	94	ARG	2
1	A	23	PHE	2
1	A	25	ARG	2
1	A	99	ARG	2
1	A	93	LEU	2
1	A	153	LEU	2
1	A	150	HIS	1
1	A	64	HIS	1
1	A	32	GLU	1
1	A	89	ARG	1
1	A	104	THR	1
1	A	46	ARG	1
1	A	92	LEU	1
1	A	60	THR	1
1	A	61	PHE	1
1	A	115	GLU	1
1	A	34	VAL	1
1	A	55	ARG	1
1	A	128	ARG	1
1	A	160	LEU	1
1	A	44	ARG	1
1	A	47	TRP	1
1	A	59	GLN	1
1	A	37	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2137
Number of shifts mapped to atoms	2137
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	-0.01 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	160	0.01 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	148	0.06 ± 0.17	None needed (< 0.5 ppm)
^{15}N	161	0.39 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1866 atoms were assigned a chemical shift out of a possible 2074. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	716/732 (98%)	297/297 (100%)	282/298 (95%)	137/137 (100%)
Sidechain	1008/1163 (87%)	691/761 (91%)	310/350 (89%)	7/52 (13%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	142/179 (79%)	78/88 (89%)	58/75 (77%)	6/16 (38%)
Overall	1866/2074 (90%)	1066/1146 (93%)	650/723 (90%)	150/205 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2137 atoms were assigned a chemical shift out of a possible 2608. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	833/942 (88%)	350/383 (91%)	322/382 (84%)	161/177 (91%)
Sidechain	1142/1403 (81%)	784/919 (85%)	350/424 (83%)	8/60 (13%)
Aromatic	162/263 (62%)	90/130 (69%)	66/101 (65%)	6/32 (19%)
Overall	2137/2608 (82%)	1224/1432 (85%)	738/907 (81%)	175/269 (65%)

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.

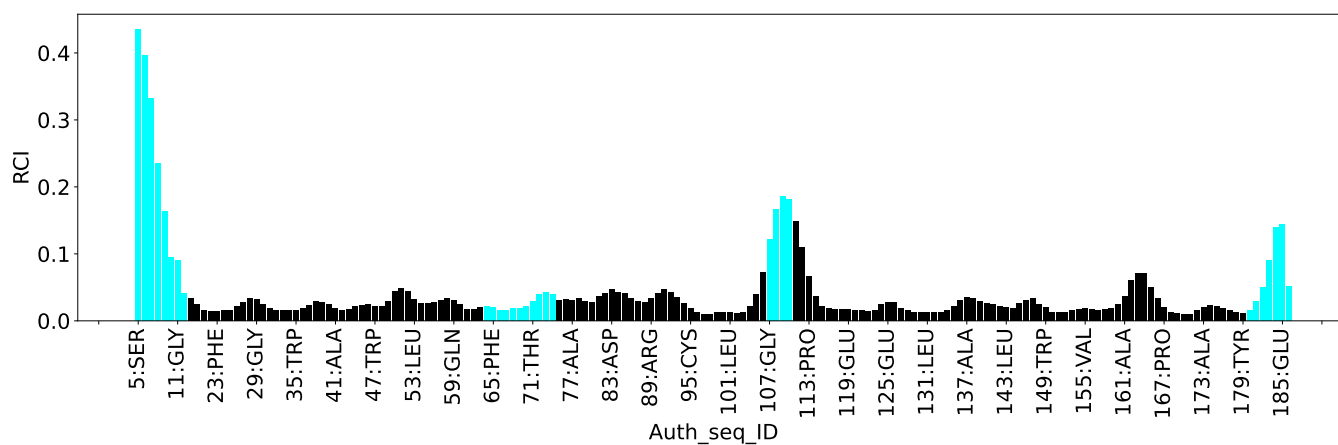
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	66	ASN	CB	9.26	30.50 – 46.89	-18.0
1	A	149	TRP	HE1	-1.28	6.88 – 13.28	-17.8
1	A	171	THR	CB	39.36	61.12 – 78.27	-17.7
1	A	170	THR	CB	40.51	61.12 – 78.27	-17.0
1	A	69	ALA	CB	47.05	10.19 – 27.75	16.0
1	A	48	LEU	HB2	-0.83	-0.07 – 3.30	-7.2
1	A	97	PRO	HA	2.27	2.78 – 6.00	-6.6
1	A	43	LYS	HB2	0.48	0.58 – 2.97	-5.5
1	A	131	LEU	HD11	-0.67	-0.61 – 2.12	-5.2
1	A	131	LEU	HD12	-0.67	-0.61 – 2.12	-5.2
1	A	131	LEU	HD13	-0.67	-0.61 – 2.12	-5.2
1	A	49	ALA	HB1	0.09	0.14 – 2.58	-5.2
1	A	49	ALA	HB2	0.09	0.14 – 2.58	-5.2
1	A	49	ALA	HB3	0.09	0.14 – 2.58	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3108
Intra-residue ($ i-j =0$)	671
Sequential ($ i-j =1$)	858
Medium range ($ i-j >1$ and $ i-j <5$)	471
Long range ($ i-j \geq 5$)	1022
Inter-chain	0
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	487
Number of unmapped restraints	0
Number of restraints per residue	18.8
Number of long range restraints per residue ¹	5.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	19.5	0.2
0.2-0.5 (Medium)	2.4	0.39
>0.5 (Large)	0.1	1.95

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)	13.8	9.31
10.0-20.0 (Medium)	0.1	10.17
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

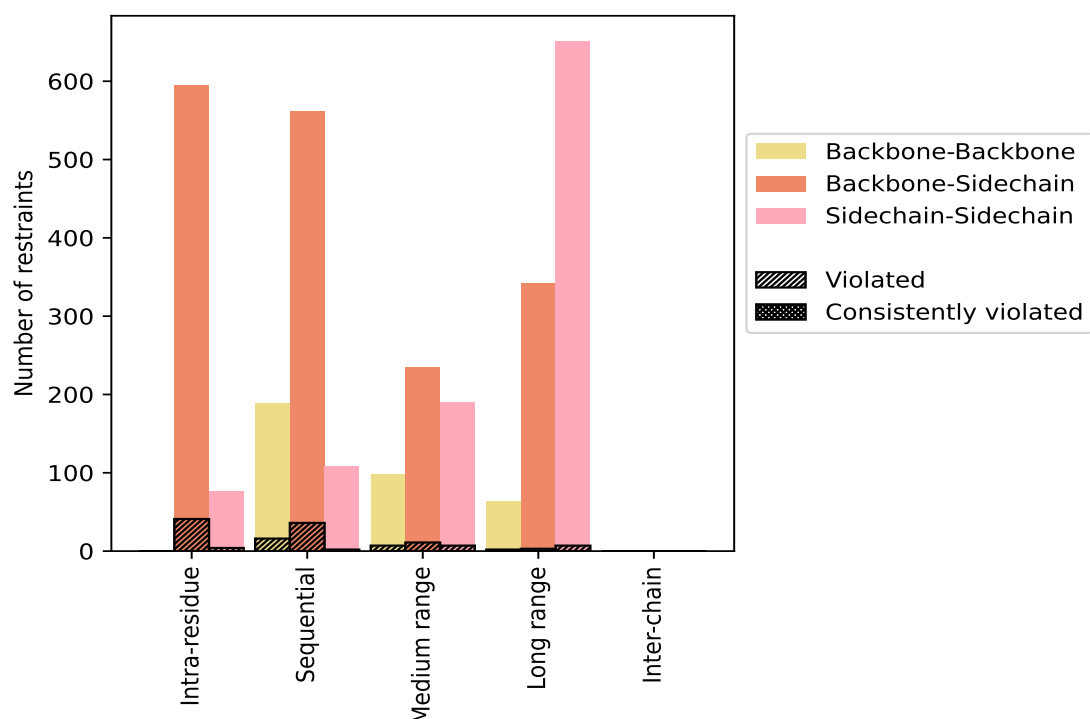
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	671	21.6	45	6.7	1.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	595	19.1	41	6.9	1.3	0	0.0	0.0
Sidechain-Sidechain	76	2.4	4	5.3	0.1	0	0.0	0.0
Sequential (i-j =1)	858	27.6	54	6.3	1.7	0	0.0	0.0
Backbone-Backbone	189	6.1	16	8.5	0.5	0	0.0	0.0
Backbone-Sidechain	561	18.1	36	6.4	1.2	0	0.0	0.0
Sidechain-Sidechain	108	3.5	2	1.9	0.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	471	15.2	21	4.5	0.7	0	0.0	0.0
Backbone-Backbone	98	3.2	7	7.1	0.2	0	0.0	0.0
Backbone-Sidechain	183	5.9	7	3.8	0.2	0	0.0	0.0
Sidechain-Sidechain	190	6.1	7	3.7	0.2	0	0.0	0.0
Long range (i-j ≥5)	1022	32.9	11	1.1	0.4	0	0.0	0.0
Backbone-Backbone	63	2.0	2	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	308	9.9	2	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	651	20.9	7	1.1	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	86	2.8	5	5.8	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3108	100.0	136	4.4	4.4	0	0.0	0.0
Backbone-Backbone	350	11.3	25	7.1	0.8	0	0.0	0.0
Backbone-Sidechain	1733	55.8	91	5.3	2.9	0	0.0	0.0
Sidechain-Sidechain	1025	33.0	20	2.0	0.6	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	10	6	4	0	0	20	0.14	0.21	0.03	0.13
2	11	6	6	1	0	24	0.15	0.22	0.04	0.14
3	8	10	6	2	0	26	0.15	0.22	0.03	0.14
4	11	13	3	2	0	29	0.14	0.26	0.04	0.13
5	4	9	4	1	0	18	0.16	0.35	0.06	0.13
6	10	6	4	0	0	20	0.16	0.36	0.06	0.14
7	10	9	3	1	0	23	0.15	0.27	0.05	0.13
8	7	10	5	1	0	23	0.15	0.25	0.04	0.14
9	10	8	6	3	0	27	0.14	0.26	0.04	0.13
10	13	6	2	0	0	21	0.15	0.25	0.05	0.12

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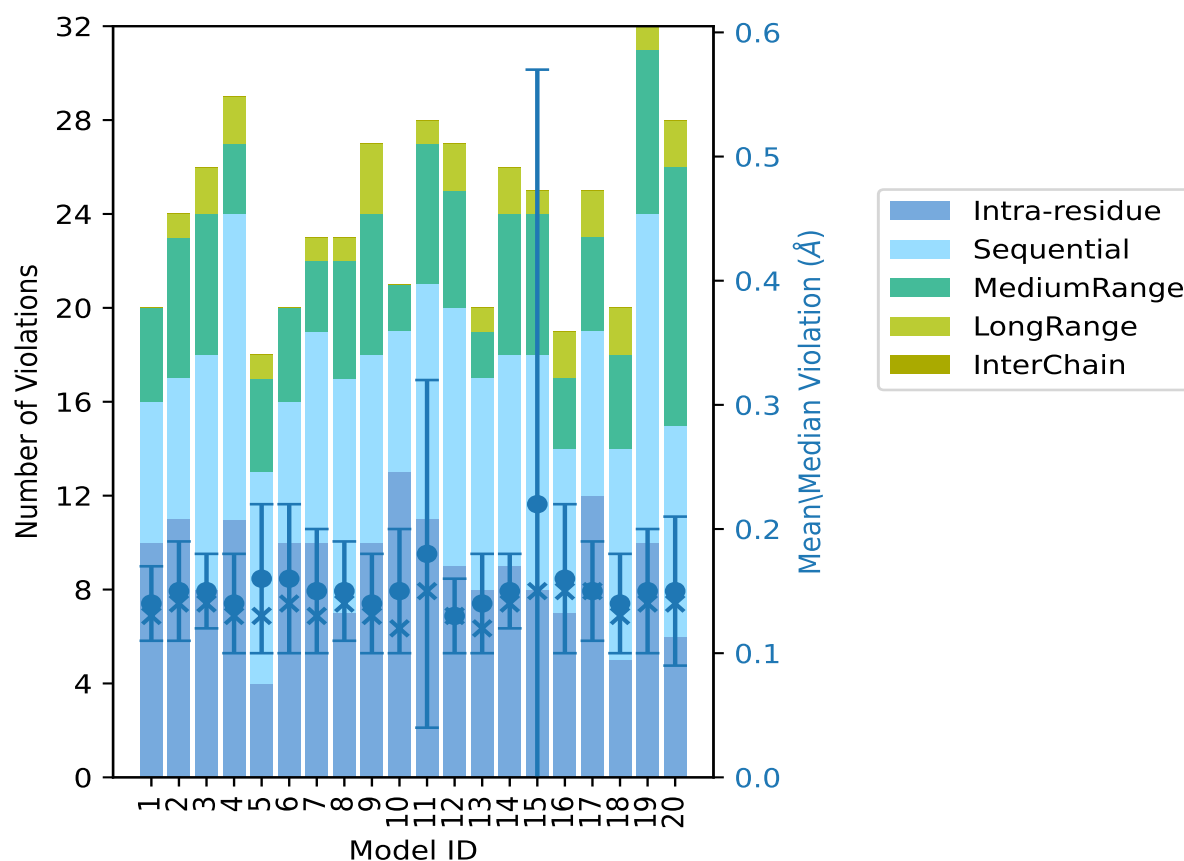
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	11	10	6	1	0	28	0.18	0.87	0.14	0.15
12	9	11	5	2	0	27	0.13	0.21	0.03	0.13
13	8	9	2	1	0	20	0.14	0.24	0.04	0.12
14	9	9	6	2	0	26	0.15	0.23	0.03	0.14
15	8	10	6	1	0	25	0.22	1.95	0.35	0.15
16	7	7	3	2	0	19	0.16	0.33	0.06	0.15
17	12	7	4	2	0	25	0.15	0.27	0.04	0.15
18	5	9	4	2	0	20	0.14	0.26	0.04	0.13
19	10	14	7	1	0	32	0.15	0.34	0.05	0.14
20	6	9	11	2	0	28	0.15	0.39	0.06	0.14

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

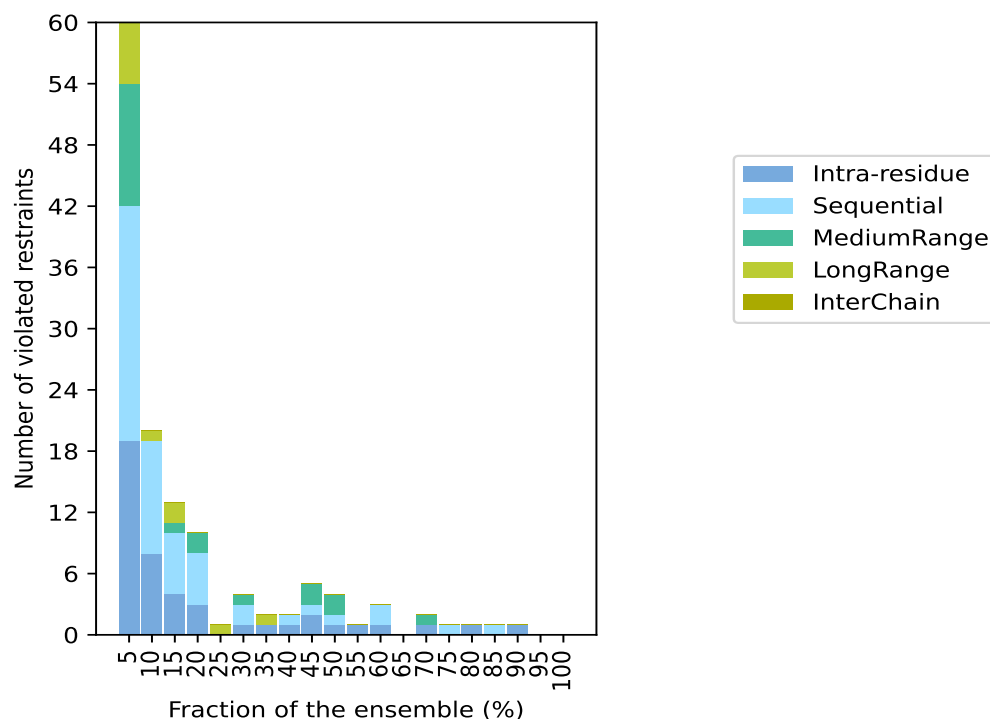
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2891(IR:626, SQ:804, MR:450, LR:1011, IC:0) restraints are 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	%
19	23	12	6	0	60	1	5.0
8	11	0	1	0	20	2	10.0
4	6	1	2	0	13	3	15.0
3	5	2	0	0	10	4	20.0
0	0	0	1	0	1	5	25.0
1	2	1	0	0	4	6	30.0
1	0	0	1	0	2	7	35.0
1	1	0	0	0	2	8	40.0
2	1	2	0	0	5	9	45.0
1	1	2	0	0	4	10	50.0
1	0	0	0	0	1	11	55.0
1	2	0	0	0	3	12	60.0
0	0	0	0	0	0	13	65.0
1	0	1	0	0	2	14	70.0
0	1	0	0	0	1	15	75.0
1	0	0	0	0	1	16	80.0
0	1	0	0	0	1	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

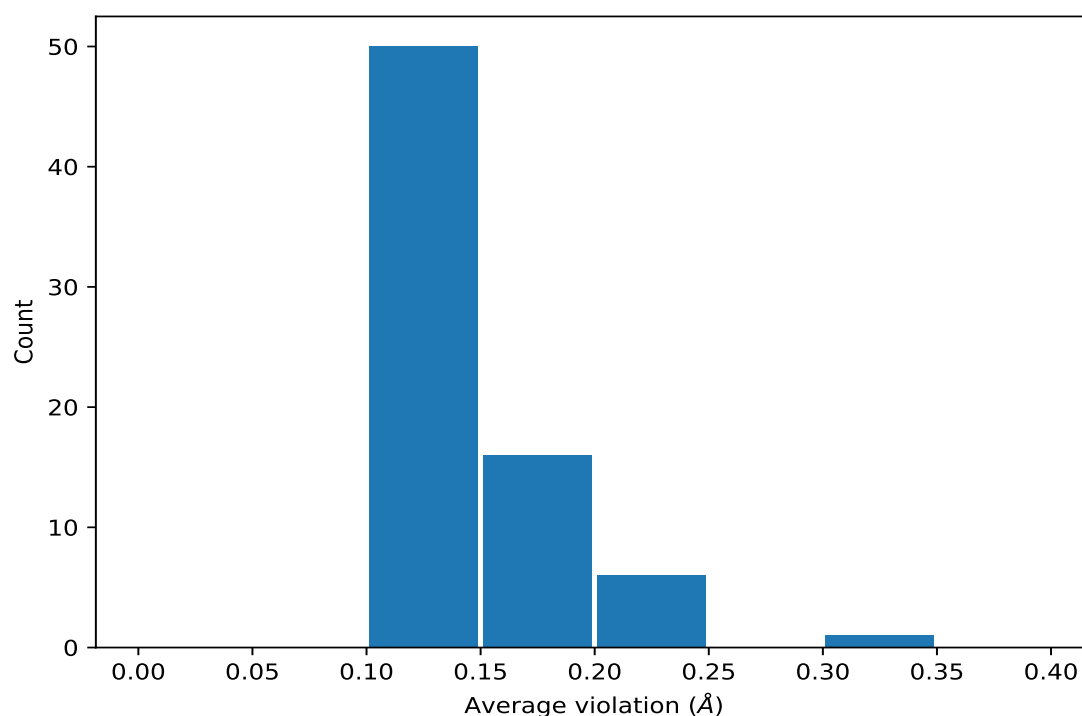
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the 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)
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	18	0.18	0.02	0.19
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	17	0.18	0.05	0.18
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	16	0.15	0.01	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	15	0.15	0.03	0.15
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	14	0.16	0.04	0.16
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	14	0.12	0.01	0.12
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	12	0.15	0.02	0.16
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	12	0.13	0.02	0.14
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	12	0.12	0.01	0.12
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	12	0.11	0.01	0.11
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	11	0.22	0.02	0.21
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	10	0.17	0.04	0.16
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	10	0.16	0.02	0.16
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	10	0.13	0.02	0.13
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	10	0.13	0.02	0.12
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	9	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	9	0.17	0.04	0.18
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	9	0.15	0.02	0.15
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	9	0.14	0.02	0.14
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	9	0.12	0.02	0.11
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	8	0.12	0.01	0.12
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	8	0.12	0.02	0.12
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	7	0.16	0.04	0.15
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	7	0.13	0.01	0.13
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	6	0.24	0.02	0.26
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	6	0.15	0.02	0.15
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	6	0.15	0.03	0.15
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	6	0.12	0.01	0.12
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	5	0.2	0.04	0.2
(2,194)	1:43:A:LYS:HE3	1:47:A:TRP:HD1	4	0.18	0.03	0.17
(1,380)	1:36:A:ALA:HA	1:40:A:ASP:H	4	0.15	0.03	0.16
(1,503)	1:122:A:GLU:HG2	1:123:A:ALA:H	4	0.14	0.01	0.14
(1,270)	1:111:A:GLU:H	1:111:A:GLU:HB3	4	0.13	0.02	0.14
(1,1203)	1:89:A:ARG:HG2	1:90:A:HIS:H	4	0.13	0.01	0.14
(1,31)	1:37:A:TRP:HB3	1:38:A:LEU:H	4	0.12	0.01	0.12
(1,46)	1:50:A:GLY:H	1:51:A:GLY:H	4	0.12	0.02	0.13
(1,892)	1:126:A:GLN:HB2	1:127:A:VAL:H	4	0.12	0.02	0.12
(1,811)	1:163:A:GLN:H	1:163:A:GLN:HB2	4	0.12	0.01	0.12
(1,1174)	1:174:A:GLN:HB3	1:174:A:GLN:HG3	4	0.1	0.0	0.1
(1,1092)	1:99:A:ARG:HB3	1:99:A:ARG:HD2	3	0.34	0.01	0.34
(2,196)	1:37:A:TRP:HE1	1:43:A:LYS:HE2	3	0.21	0.13	0.13
(1,129)	1:107:A:GLY:H	1:108:A:GLY:H	3	0.19	0.03	0.2
(1,798)	1:127:A:VAL:H	1:127:A:VAL:HB	3	0.17	0.04	0.18
(1,850)	1:49:A:ALA:HA	1:50:A:GLY:H	3	0.17	0.01	0.17
(1,943)	1:96:A:GLU:H	1:100:A:VAL:HB	3	0.17	0.06	0.14
(1,784)	1:99:A:ARG:H	1:99:A:ARG:HB3	3	0.14	0.03	0.13
(1,260)	1:82:A:TYR:H	1:82:A:TYR:HB2	3	0.14	0.01	0.14
(2,59)	1:37:A:TRP:HE1	1:43:A:LYS:HD2	3	0.14	0.01	0.13
(1,50)	1:51:A:GLY:HA3	1:52:A:GLU:H	3	0.13	0.02	0.13
(1,161)	1:128:A:ARG:HB2	1:129:A:LEU:H	3	0.13	0.02	0.12
(1,138)	1:117:A:LEU:HB2	1:118:A:PHE:H	3	0.12	0.02	0.12
(1,127)	1:104:A:THR:HB	1:105:A:TRP:H	3	0.11	0.0	0.11
(1,1108)	1:115:A:GLU:HA	1:115:A:GLU:HG3	2	0.23	0.02	0.23
(1,507)	1:25:A:ARG:H	1:25:A:ARG:HG2	2	0.2	0.04	0.2
(1,548)	1:182:A:ARG:H	1:182:A:ARG:HG3	2	0.18	0.0	0.18
(1,1139)	1:139:A:ARG:HA	1:139:A:ARG:HG3	2	0.17	0.01	0.17
(1,1148)	1:143:A:LEU:H	1:143:A:LEU:HG	2	0.16	0.02	0.16
(1,130)	1:111:A:GLU:HB2	1:112:A:ALA:H	2	0.15	0.02	0.15

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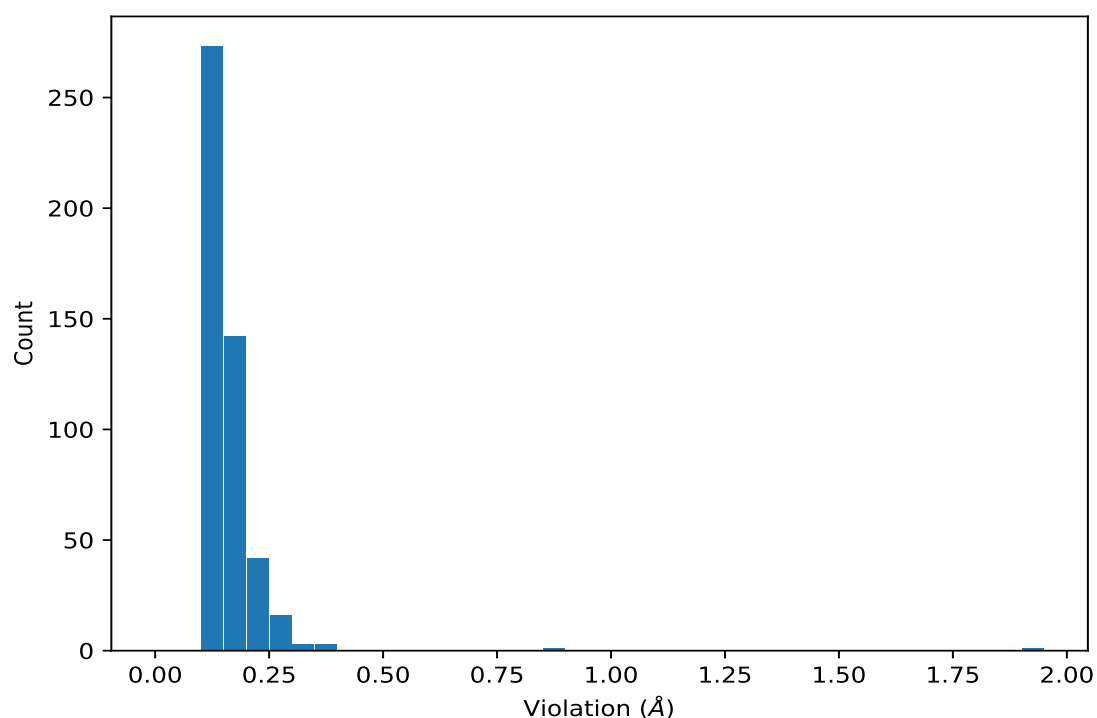
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1141)	1:139:A:ARG:HA	1:139:A:ARG:HD2	2	0.15	0.03	0.15
(2,54)	1:126:A:GLN:HE22	1:127:A:VAL:H	2	0.14	0.03	0.14
(1,859)	1:65:A:PHE:HA	1:66:A:ASN:H	2	0.14	0.04	0.14
(1,497)	1:48:A:LEU:HG	1:49:A:ALA:H	2	0.14	0.01	0.14
(1,250)	1:53:A:LEU:H	1:53:A:LEU:HB3	2	0.13	0.03	0.13
(1,94)	1:81:A:GLN:H	1:82:A:TYR:H	2	0.12	0.02	0.12
(1,508)	1:25:A:ARG:H	1:25:A:ARG:HG3	2	0.12	0.01	0.12
(1,1198)	1:52:A:GLU:HG3	1:53:A:LEU:H	2	0.12	0.01	0.12
(1,326)	1:86:A:ILE:H	1:87:A:VAL:H	2	0.12	0.02	0.12
(1,894)	1:128:A:ARG:HB3	1:129:A:LEU:H	2	0.11	0.01	0.11
(1,919)	1:181:A:GLN:HB2	1:182:A:ARG:H	2	0.11	0.01	0.11
(2,164)	1:128:A:ARG:HD2	1:129:A:LEU:H	2	0.11	0.0	0.11
(3,55)	1:149:A:TRP:O	1:152:A:HIS:H	2	0.11	0.01	0.11
(1,1216)	1:131:A:LEU:HG	1:132:A:THR:H	2	0.11	0.0	0.11
(1,1284)	1:119:A:GLU:H	1:130:A:VAL:HB	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table 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)
(1,549)	1:44:A:ARG:HA	1:47:A:TRP:HE1	15	1.95
(1,449)	1:167:A:PRO:HA	1:169:A:TRP:H	11	0.87
(2,196)	1:37:A:TRP:HE1	1:43:A:LYS:HE2	20	0.39
(1,1117)	1:122:A:GLU:HA	1:122:A:GLU:HG3	6	0.36
(1,1092)	1:99:A:ARG:HB3	1:99:A:ARG:HD2	5	0.35
(1,1241)	1:37:A:TRP:HA	1:43:A:LYS:HB3	19	0.34
(1,1092)	1:99:A:ARG:HB3	1:99:A:ARG:HD2	11	0.34
(1,1092)	1:99:A:ARG:HB3	1:99:A:ARG:HD2	16	0.33
(1,771)	1:70:A:LEU:H	1:70:A:LEU:HB3	17	0.27
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	7	0.27
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	16	0.27
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	4	0.26
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	9	0.26
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	18	0.26
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	15	0.25
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:115:A:GLU:HA	1:115:A:GLU:HG3	7	0.25
(1,943)	1:96:A:GLU:H	1:100:A:VAL:HB	8	0.25
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	15	0.25
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	19	0.25
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	7	0.25
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	17	0.25
(1,507)	1:25:A:ARG:H	1:25:A:ARG:HG2	10	0.25
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	20	0.25
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	8	0.24
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	13	0.24
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	6	0.23
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	4	0.23
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	10	0.23
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	14	0.23
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	11	0.23
(2,194)	1:43:A:LYS:HE3	1:47:A:TRP:HD1	3	0.22
(1,798)	1:127:A:VAL:H	1:127:A:VAL:HB	2	0.22
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	10	0.22
(1,785)	1:100:A:VAL:H	1:100:A:VAL:HB	17	0.22
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	9	0.22
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	1	0.21
(1,1108)	1:115:A:GLU:HA	1:115:A:GLU:HG3	12	0.21
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	9	0.21
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	5	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	1	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	4	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	6	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	13	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	14	0.21
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	18	0.21
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	2	0.21
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	19	0.21
(1,129)	1:107:A:GLY:H	1:108:A:GLY:H	5	0.21
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	2	0.2
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	5	0.2
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	7	0.2
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	10	0.2
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	15	0.2
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	2	0.2
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	3	0.2
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	6	0.2
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	10	0.2
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	12	0.2
(1,761)	1:52:A:GLU:H	1:52:A:GLU:HB2	3	0.2
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	5	0.2
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	6	0.2
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	1	0.2
(1,129)	1:107:A:GLY:H	1:108:A:GLY:H	8	0.2
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	2	0.2
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	4	0.19
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	16	0.19
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	3	0.19
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	6	0.19
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	11	0.19
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	14	0.19
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	16	0.19
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	20	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	4	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	8	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	13	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	15	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	16	0.19
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	17	0.19
(1,380)	1:36:A:ALA:HA	1:40:A:ASP:H	20	0.19
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	10	0.19
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	15	0.19
(1,49)	1:51:A:GLY:HA2	1:52:A:GLU:H	3	0.19
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	11	0.18
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	19	0.18
(2,144)	1:55:A:ARG:HD2	1:56:A:GLN:H	14	0.18
(2,54)	1:126:A:GLN:HE22	1:127:A:VAL:H	19	0.18
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	1	0.18
(1,1148)	1:143:A:LEU:H	1:143:A:LEU:HG	20	0.18
(1,1139)	1:139:A:ARG:HA	1:139:A:ARG:HG3	19	0.18
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	9	0.18
(1,859)	1:65:A:PHE:HA	1:66:A:ASN:H	9	0.18
(1,850)	1:49:A:ALA:HA	1:50:A:GLY:H	5	0.18
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	4	0.18
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	9	0.18
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	17	0.18
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	1	0.18
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	2	0.18
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,798)	1:127:A:VAL:H	1:127:A:VAL:HB	3	0.18
(1,784)	1:99:A:ARG:H	1:99:A:ARG:HB3	14	0.18
(1,548)	1:182:A:ARG:H	1:182:A:ARG:HG3	16	0.18
(1,547)	1:182:A:ARG:H	1:182:A:ARG:HG2	14	0.18
(1,478)	1:71:A:THR:HB	1:72:A:ALA:H	18	0.18
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	17	0.18
(1,287)	1:149:A:TRP:H	1:149:A:TRP:HB3	20	0.18
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	6	0.18
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	8	0.18
(2,194)	1:43:A:LYS:HE3	1:47:A:TRP:HD1	7	0.17
(2,194)	1:43:A:LYS:HE3	1:47:A:TRP:HD1	17	0.17
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	2	0.17
(1,1242)	1:43:A:LYS:HD3	1:47:A:TRP:HD1	20	0.17
(1,1141)	1:139:A:ARG:HA	1:139:A:ARG:HD2	17	0.17
(1,1103)	1:111:A:GLU:HB2	1:111:A:GLU:HG3	13	0.17
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	20	0.17
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	5	0.17
(1,850)	1:49:A:ALA:HA	1:50:A:GLY:H	11	0.17
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	15	0.17
(1,806)	1:144:A:ASP:H	1:144:A:ASP:HB3	4	0.17
(1,548)	1:182:A:ARG:H	1:182:A:ARG:HG3	19	0.17
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	16	0.17
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	19	0.17
(1,248)	1:52:A:GLU:H	1:52:A:GLU:HB3	11	0.17
(1,130)	1:111:A:GLU:HB2	1:112:A:ALA:H	11	0.17
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	17	0.17
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	17	0.16
(2,59)	1:37:A:TRP:HE1	1:43:A:LYS:HD2	13	0.16
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	4	0.16
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	8	0.16
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	3	0.16
(1,1243)	1:43:A:LYS:HD2	1:47:A:TRP:HD1	19	0.16
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	13	0.16
(1,1139)	1:139:A:ARG:HA	1:139:A:ARG:HG3	12	0.16
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	17	0.16
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	8	0.16
(1,850)	1:49:A:ALA:HA	1:50:A:GLY:H	9	0.16
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	1	0.16
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	8	0.16
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	18	0.16
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	16	0.16
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:25:A:ARG:H	1:25:A:ARG:HG2	2	0.16
(1,503)	1:122:A:GLU:HG2	1:123:A:ALA:H	3	0.16
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	11	0.16
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	1	0.16
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	14	0.16
(1,386)	1:43:A:LYS:H	1:45:A:ALA:H	15	0.16
(1,380)	1:36:A:ALA:HA	1:40:A:ASP:H	9	0.16
(1,250)	1:53:A:LEU:H	1:53:A:LEU:HB3	3	0.16
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	6	0.16
(1,161)	1:128:A:ARG:HB2	1:129:A:LEU:H	19	0.16
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	4	0.16
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	10	0.16
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	14	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	4	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	8	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	10	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	12	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	16	0.16
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	17	0.16
(1,50)	1:51:A:GLY:HA3	1:52:A:GLU:H	4	0.16
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	9	0.15
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	20	0.15
(2,194)	1:43:A:LYS:HE3	1:47:A:TRP:HD1	20	0.15
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	14	0.15
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	15	0.15
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	8	0.15
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	11	0.15
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	15	0.15
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	6	0.15
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	11	0.15
(1,892)	1:126:A:GLN:HB2	1:127:A:VAL:H	7	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	7	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	14	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	15	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	16	0.15
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	17	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	2	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	3	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	4	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	6	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	7	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	9	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	10	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	11	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	12	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	13	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	14	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	15	0.15
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	19	0.15
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	10	0.15
(1,503)	1:122:A:GLU:HG2	1:123:A:ALA:H	11	0.15
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	15	0.15
(1,380)	1:36:A:ALA:HA	1:40:A:ASP:H	12	0.15
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	5	0.15
(1,363)	1:182:A:ARG:H	1:183:A:LEU:H	14	0.15
(1,270)	1:111:A:GLU:H	1:111:A:GLU:HB3	1	0.15
(1,260)	1:82:A:TYR:H	1:82:A:TYR:HB2	11	0.15
(1,245)	1:40:A:ASP:HB2	1:43:A:LYS:H	3	0.15
(1,207)	1:168:A:PHE:H	1:169:A:TRP:H	11	0.15
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	3	0.15
(1,129)	1:107:A:GLY:H	1:108:A:GLY:H	18	0.15
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	19	0.15
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	12	0.15
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	19	0.15
(1,48)	1:50:A:GLY:HA3	1:51:A:GLY:H	19	0.15
(1,1276)	1:104:A:THR:HB	1:115:A:GLU:HB3	9	0.14
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	5	0.14
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	7	0.14
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	12	0.14
(1,1203)	1:89:A:ARG:HG2	1:90:A:HIS:H	16	0.14
(1,1203)	1:89:A:ARG:HG2	1:90:A:HIS:H	20	0.14
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	11	0.14
(1,943)	1:96:A:GLU:H	1:100:A:VAL:HB	19	0.14
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	8	0.14
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	19	0.14
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	12	0.14
(1,854)	1:55:A:ARG:HB3	1:56:A:GLN:H	15	0.14
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	3	0.14
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	20	0.14
(1,811)	1:163:A:GLN:H	1:163:A:GLN:HB2	12	0.14
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	2	0.14
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	18	0.14
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,497)	1:48:A:LEU:HG	1:49:A:ALA:H	4	0.14
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	12	0.14
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	20	0.14
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	1	0.14
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	2	0.14
(1,270)	1:111:A:GLU:H	1:111:A:GLU:HB3	8	0.14
(1,260)	1:82:A:TYR:H	1:82:A:TYR:HB2	3	0.14
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	4	0.14
(1,138)	1:117:A:LEU:HB2	1:118:A:PHE:H	12	0.14
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	3	0.14
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	14	0.14
(1,94)	1:81:A:GLN:H	1:82:A:TYR:H	7	0.14
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	3	0.14
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	20	0.14
(1,46)	1:50:A:GLY:H	1:51:A:GLY:H	3	0.14
(1,46)	1:50:A:GLY:H	1:51:A:GLY:H	17	0.14
(1,31)	1:37:A:TRP:HB3	1:38:A:LEU:H	18	0.14
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	6	0.13
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	18	0.13
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	20	0.13
(3,25)	1:115:A:GLU:H	1:134:A:THR:O	7	0.13
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	2	0.13
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	18	0.13
(2,196)	1:37:A:TRP:HE1	1:43:A:LYS:HE2	12	0.13
(2,62)	1:56:A:GLN:HG2	1:59:A:GLN:HE21	20	0.13
(2,59)	1:37:A:TRP:HE1	1:43:A:LYS:HD2	9	0.13
(2,59)	1:37:A:TRP:HE1	1:43:A:LYS:HD2	14	0.13
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	17	0.13
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	11	0.13
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	14	0.13
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	18	0.13
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	2	0.13
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	18	0.13
(1,1203)	1:89:A:ARG:HG2	1:90:A:HIS:H	9	0.13
(1,1198)	1:52:A:GLU:HG3	1:53:A:LEU:H	3	0.13
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	12	0.13
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	15	0.13
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	19	0.13
(1,1148)	1:143:A:LEU:H	1:143:A:LEU:HG	19	0.13
(1,1087)	1:96:A:GLU:HA	1:96:A:GLU:HG3	19	0.13
(1,1038)	1:55:A:ARG:H	1:55:A:ARG:HG3	20	0.13
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	18	0.13
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	6	0.13
(1,939)	1:79:A:TYR:H	1:80:A:ALA:HA	12	0.13
(1,892)	1:126:A:GLN:HB2	1:127:A:VAL:H	15	0.13
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	1	0.13
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	13	0.13
(1,833)	1:9:A:PRO:HB2	1:10:A:ASP:H	8	0.13
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	2	0.13
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	7	0.13
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	1	0.13
(1,816)	1:174:A:GLN:HA	1:174:A:GLN:HB3	16	0.13
(1,811)	1:163:A:GLN:H	1:163:A:GLN:HB2	7	0.13
(1,784)	1:99:A:ARG:H	1:99:A:ARG:HB3	7	0.13
(1,781)	1:87:A:VAL:H	1:87:A:VAL:HB	2	0.13
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	6	0.13
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	14	0.13
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	19	0.13
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	11	0.13
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	13	0.13
(1,508)	1:25:A:ARG:H	1:25:A:ARG:HG3	13	0.13
(1,503)	1:122:A:GLU:HG2	1:123:A:ALA:H	4	0.13
(1,503)	1:122:A:GLU:HG2	1:123:A:ALA:H	18	0.13
(1,497)	1:48:A:LEU:HG	1:49:A:ALA:H	3	0.13
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	3	0.13
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	18	0.13
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	2	0.13
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	14	0.13
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	15	0.13
(1,351)	1:149:A:TRP:H	1:150:A:HIS:H	20	0.13
(1,326)	1:86:A:ILE:H	1:87:A:VAL:H	14	0.13
(1,300)	1:169:A:TRP:H	1:169:A:TRP:HB3	11	0.13
(1,270)	1:111:A:GLU:H	1:111:A:GLU:HB3	7	0.13
(1,260)	1:82:A:TYR:H	1:82:A:TYR:HB2	12	0.13
(1,183)	1:145:A:VAL:HB	1:146:A:ALA:H	20	0.13
(1,130)	1:111:A:GLU:HB2	1:112:A:ALA:H	16	0.13
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	16	0.13
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	1	0.13
(1,50)	1:51:A:GLY:HA3	1:52:A:GLU:H	19	0.13
(3,55)	1:149:A:TRP:O	1:152:A:HIS:H	18	0.12
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	9	0.12
(3,11)	1:44:A:ARG:O	1:48:A:LEU:H	15	0.12
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,242)	1:104:A:THR:HB	1:115:A:GLU:HG3	14	0.12
(2,195)	1:37:A:TRP:HE1	1:43:A:LYS:HE3	9	0.12
(1,1310)	1:177:A:GLN:HA	1:180:A:GLU:HG2	20	0.12
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	12	0.12
(1,1290)	1:145:A:VAL:HB	1:149:A:TRP:HE1	19	0.12
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	12	0.12
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	13	0.12
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	8	0.12
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	9	0.12
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	20	0.12
(1,1170)	1:174:A:GLN:HB3	1:174:A:GLN:HG2	18	0.12
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	6	0.12
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	8	0.12
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	10	0.12
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	14	0.12
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	15	0.12
(1,1141)	1:139:A:ARG:HA	1:139:A:ARG:HD2	10	0.12
(1,1049)	1:59:A:GLN:HA	1:59:A:GLN:HG2	17	0.12
(1,997)	1:19:A:GLN:HA	1:19:A:GLN:HG3	9	0.12
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	9	0.12
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	19	0.12
(1,943)	1:96:A:GLU:H	1:100:A:VAL:HB	20	0.12
(1,919)	1:181:A:GLN:HB2	1:182:A:ARG:H	4	0.12
(1,898)	1:139:A:ARG:HB3	1:140:A:ALA:H	17	0.12
(1,894)	1:128:A:ARG:HB3	1:129:A:LEU:H	4	0.12
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	18	0.12
(1,844)	1:28:A:PRO:HB3	1:29:A:GLY:H	3	0.12
(1,827)	1:180:A:GLU:H	1:180:A:GLU:HB3	10	0.12
(1,798)	1:127:A:VAL:H	1:127:A:VAL:HB	17	0.12
(1,784)	1:99:A:ARG:H	1:99:A:ARG:HB3	1	0.12
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	1	0.12
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	12	0.12
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	19	0.12
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	1	0.12
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	5	0.12
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	10	0.12
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	13	0.12
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	12	0.12
(1,524)	1:52:A:GLU:H	1:52:A:GLU:HG2	8	0.12
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	4	0.12
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	15	0.12
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:123:A:ALA:HA	1:126:A:GLN:H	8	0.12
(1,422)	1:123:A:ALA:H	1:128:A:ARG:H	3	0.12
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	11	0.12
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	20	0.12
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	2	0.12
(1,161)	1:128:A:ARG:HB2	1:129:A:LEU:H	13	0.12
(1,138)	1:117:A:LEU:HB2	1:118:A:PHE:H	16	0.12
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	7	0.12
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	15	0.12
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	5	0.12
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	18	0.12
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	1	0.12
(1,46)	1:50:A:GLY:H	1:51:A:GLY:H	14	0.12
(1,31)	1:37:A:TRP:HB3	1:38:A:LEU:H	13	0.12
(1,31)	1:37:A:TRP:HB3	1:38:A:LEU:H	14	0.12
(1,31)	1:37:A:TRP:HB3	1:38:A:LEU:H	17	0.12
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	3	0.11
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	5	0.11
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	7	0.11
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	12	0.11
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	13	0.11
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	14	0.11
(2,248)	1:31:A:ILE:HG12	1:122:A:GLU:HB2	12	0.11
(2,196)	1:37:A:TRP:HE1	1:43:A:LYS:HE2	16	0.11
(2,165)	1:128:A:ARG:HD3	1:129:A:LEU:H	10	0.11
(2,164)	1:128:A:ARG:HD2	1:129:A:LEU:H	2	0.11
(2,164)	1:128:A:ARG:HD2	1:129:A:LEU:H	7	0.11
(2,145)	1:55:A:ARG:HD3	1:56:A:GLN:H	13	0.11
(2,60)	1:37:A:TRP:HE1	1:43:A:LYS:HD3	17	0.11
(2,54)	1:126:A:GLN:HE22	1:127:A:VAL:H	11	0.11
(1,1284)	1:119:A:GLU:H	1:130:A:VAL:HB	4	0.11
(1,1257)	1:56:A:GLN:HG3	1:59:A:GLN:HG3	17	0.11
(1,1255)	1:56:A:GLN:HG3	1:57:A:PRO:HD3	6	0.11
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	1	0.11
(1,1216)	1:131:A:LEU:HG	1:132:A:THR:H	6	0.11
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	6	0.11
(1,1203)	1:89:A:ARG:HG2	1:90:A:HIS:H	19	0.11
(1,1198)	1:52:A:GLU:HG3	1:53:A:LEU:H	11	0.11
(1,1194)	1:21:A:ILE:HG13	1:22:A:ARG:H	4	0.11
(1,1177)	1:176:A:GLU:H	1:176:A:GLU:HG3	14	0.11
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	1	0.11
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	4	0.11
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	7	0.11
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	9	0.11
(1,1167)	1:174:A:GLN:H	1:174:A:GLN:HG2	11	0.11
(1,1031)	1:52:A:GLU:H	1:52:A:GLU:HG3	5	0.11
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	2	0.11
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	14	0.11
(1,962)	1:173:A:ALA:HA	1:176:A:GLU:HB3	8	0.11
(1,892)	1:126:A:GLN:HB2	1:127:A:VAL:H	5	0.11
(1,892)	1:126:A:GLN:HB2	1:127:A:VAL:H	13	0.11
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	5	0.11
(1,887)	1:121:A:SER:HB2	1:122:A:GLU:H	19	0.11
(1,829)	1:181:A:GLN:HA	1:181:A:GLN:HB2	9	0.11
(1,821)	1:176:A:GLU:H	1:176:A:GLU:HB3	7	0.11
(1,819)	1:174:A:GLN:H	1:174:A:GLN:HB3	17	0.11
(1,811)	1:163:A:GLN:H	1:163:A:GLN:HB2	9	0.11
(1,811)	1:163:A:GLN:H	1:163:A:GLN:HB2	14	0.11
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	2	0.11
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	9	0.11
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	15	0.11
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	20	0.11
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	4	0.11
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	11	0.11
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	12	0.11
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	17	0.11
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	1	0.11
(1,767)	1:56:A:GLN:H	1:56:A:GLN:HB3	6	0.11
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	6	0.11
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	10	0.11
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	19	0.11
(1,508)	1:25:A:ARG:H	1:25:A:ARG:HG3	17	0.11
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	13	0.11
(1,350)	1:147:A:GLY:H	1:148:A:GLY:H	8	0.11
(1,320)	1:69:A:ALA:H	1:70:A:LEU:H	12	0.11
(1,188)	1:150:A:HIS:HB3	1:151:A:ALA:H	5	0.11
(1,161)	1:128:A:ARG:HB2	1:129:A:LEU:H	4	0.11
(1,127)	1:104:A:THR:HB	1:105:A:TRP:H	7	0.11
(1,127)	1:104:A:THR:HB	1:105:A:TRP:H	10	0.11
(1,127)	1:104:A:THR:HB	1:105:A:TRP:H	12	0.11
(1,97)	1:83:A:ASP:HA	1:84:A:ARG:H	12	0.11
(1,94)	1:81:A:GLN:H	1:82:A:TYR:H	10	0.11
(1,91)	1:78:A:ARG:HB2	1:79:A:TYR:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	15	0.11
(1,65)	1:61:A:PHE:HB3	1:62:A:GLU:H	19	0.11
(1,50)	1:51:A:GLY:HA3	1:52:A:GLU:H	15	0.11
(3,55)	1:149:A:TRP:O	1:152:A:HIS:H	8	0.1
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	10	0.1
(3,49)	1:141:A:ALA:O	1:144:A:ASP:H	11	0.1
(3,47)	1:140:A:ALA:O	1:144:A:ASP:H	9	0.1
(2,316)	1:43:A:LYS:HE2	1:47:A:TRP:HD1	16	0.1
(1,1284)	1:119:A:GLU:H	1:130:A:VAL:HB	18	0.1
(1,1254)	1:56:A:GLN:HG3	1:57:A:PRO:HD2	19	0.1
(1,1216)	1:131:A:LEU:HG	1:132:A:THR:H	8	0.1
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	3	0.1
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	9	0.1
(1,1214)	1:126:A:GLN:HG3	1:127:A:VAL:H	20	0.1
(1,1213)	1:126:A:GLN:HG2	1:127:A:VAL:H	19	0.1
(1,1174)	1:174:A:GLN:HB3	1:174:A:GLN:HG3	2	0.1
(1,1174)	1:174:A:GLN:HB3	1:174:A:GLN:HG3	4	0.1
(1,1174)	1:174:A:GLN:HB3	1:174:A:GLN:HG3	6	0.1
(1,1174)	1:174:A:GLN:HB3	1:174:A:GLN:HG3	10	0.1
(1,989)	1:178:A:ASP:HA	1:181:A:GLN:HB3	9	0.1
(1,965)	1:174:A:GLN:HA	1:177:A:GLN:HB3	12	0.1
(1,919)	1:181:A:GLN:HB2	1:182:A:ARG:H	13	0.1
(1,914)	1:177:A:GLN:HB3	1:178:A:ASP:H	2	0.1
(1,906)	1:171:A:THR:HB	1:172:A:LEU:H	20	0.1
(1,894)	1:128:A:ARG:HB3	1:129:A:LEU:H	19	0.1
(1,863)	1:83:A:ASP:HB2	1:84:A:ARG:H	9	0.1
(1,859)	1:65:A:PHE:HA	1:66:A:ASN:H	5	0.1
(1,782)	1:89:A:ARG:H	1:89:A:ARG:HB2	13	0.1
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	15	0.1
(1,772)	1:74:A:THR:HA	1:74:A:THR:HB	16	0.1
(1,768)	1:60:A:THR:H	1:60:A:THR:HB	17	0.1
(1,513)	1:37:A:TRP:H	1:37:A:TRP:HE1	8	0.1
(1,431)	1:138:A:ASP:H	1:142:A:MET:H	20	0.1
(1,412)	1:105:A:TRP:H	1:114:A:SER:H	4	0.1
(1,400)	1:77:A:ALA:HA	1:80:A:ALA:H	10	0.1
(1,380)	1:36:A:ALA:HA	1:40:A:ASP:H	16	0.1
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	3	0.1
(1,374)	1:37:A:TRP:H	1:39:A:ALA:H	4	0.1
(1,326)	1:86:A:ILE:H	1:87:A:VAL:H	4	0.1
(1,270)	1:111:A:GLU:H	1:111:A:GLU:HB3	4	0.1
(1,250)	1:53:A:LEU:H	1:53:A:LEU:HB3	20	0.1
(1,187)	1:150:A:HIS:HB2	1:151:A:ALA:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:117:A:LEU:HB2	1:118:A:PHE:H	18	0.1
(1,89)	1:74:A:THR:HB	1:75:A:ALA:H	4	0.1
(1,46)	1:50:A:GLY:H	1:51:A:GLY:H	7	0.1

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

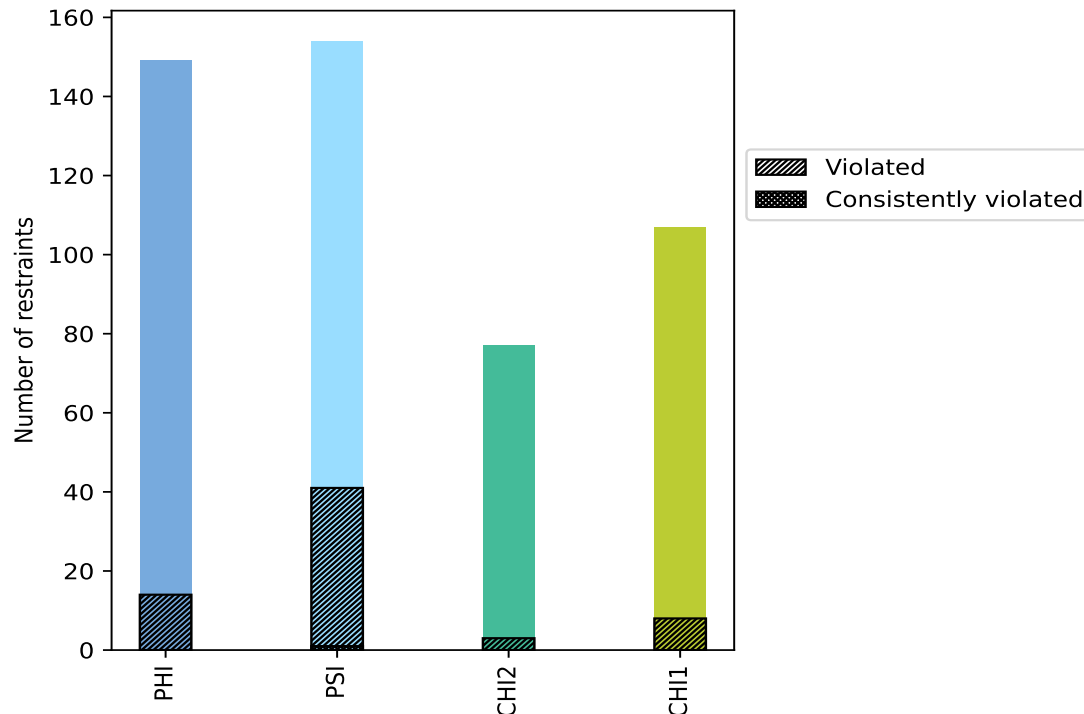
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	149	30.6	14	9.4	2.9	0	0.0	0.0
PSI	154	31.6	41	26.6	8.4	1	0.6	0.2
CHI2	77	15.8	3	3.9	0.6	0	0.0	0.0
CHI1	107	22.0	8	7.5	1.6	0	0.0	0.0
Total	487	100.0	66	13.6	13.6	1	0.2	0.2

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 [i](#)



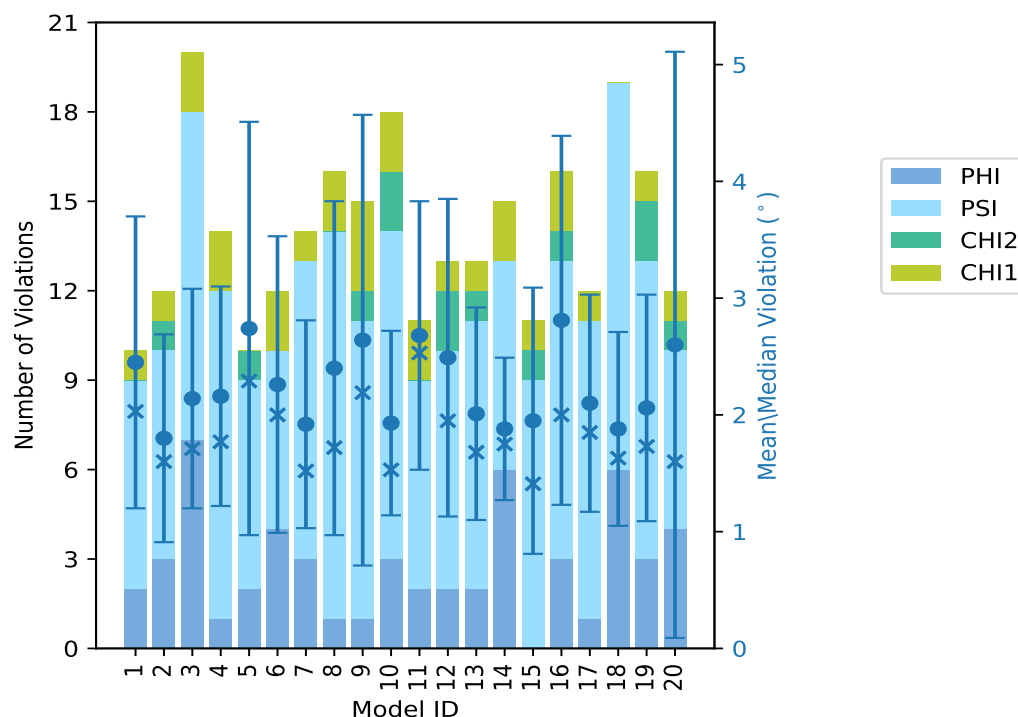
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations					Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	CHI2	CHI1	Total				
1	2	7	0	1	10	2.45	4.73	1.25	2.03
2	3	7	1	1	12	1.8	4.57	0.89	1.6
3	7	11	0	2	20	2.14	4.56	0.94	1.71
4	1	11	0	2	14	2.16	4.05	0.94	1.77
5	2	7	1	0	10	2.74	7.17	1.77	2.29
6	4	6	0	2	12	2.26	5.89	1.27	2.0
7	3	10	0	1	14	1.92	3.74	0.89	1.52
8	1	13	0	2	16	2.4	6.59	1.43	1.72
9	1	10	1	3	15	2.64	9.31	1.93	2.19
10	3	11	2	2	18	1.93	3.65	0.79	1.53
11	2	7	0	2	11	2.68	4.48	1.15	2.53
12	2	8	2	1	13	2.49	5.59	1.36	1.95
13	2	9	1	1	13	2.01	4.17	0.91	1.68
14	6	7	0	2	15	1.88	3.04	0.61	1.75
15	0	9	1	1	11	1.95	5.25	1.14	1.41
16	3	10	1	2	16	2.81	7.01	1.58	2.0
17	1	10	0	1	12	2.1	4.39	0.93	1.85
18	6	13	0	0	19	1.88	3.96	0.83	1.63
19	3	10	2	1	16	2.06	4.39	0.97	1.73
20	4	6	1	1	12	2.6	10.17	2.51	1.6

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 [i](#)

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

Number of violated restraints					Fraction of the ensemble	
PHI	PSI	CHI2	CHI1	Total	Count ¹	%
3	16	0	5	24	1	5.0
1	6	1	1	9	2	10.0
3	5	1	0	9	3	15.0
3	3	0	0	6	4	20.0
2	1	0	0	3	5	25.0
1	0	0	0	1	6	30.0
0	2	0	0	2	7	35.0
0	0	1	1	2	8	40.0
0	2	0	0	2	9	45.0
0	0	0	0	0	10	50.0
0	0	0	0	0	11	55.0

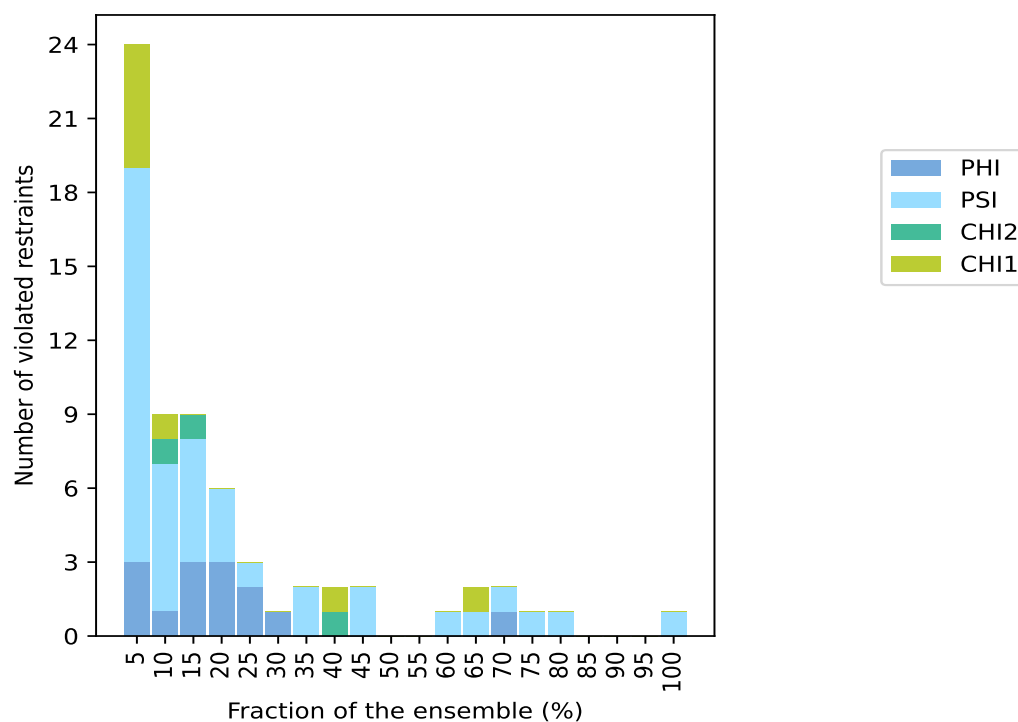
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Number of violated restraints					Fraction of the ensemble	
PHI	PSI	CHI2	CHI1	Total	Count ¹	%
0	1	0	0	1	12	60.0
0	1	0	1	2	13	65.0
1	1	0	0	2	14	70.0
0	1	0	0	1	15	75.0
0	1	0	0	1	16	80.0
0	0	0	0	0	17	85.0
0	0	0	0	0	18	90.0
0	0	0	0	0	19	95.0
0	1	0	0	1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

¹ Number of models with violations

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

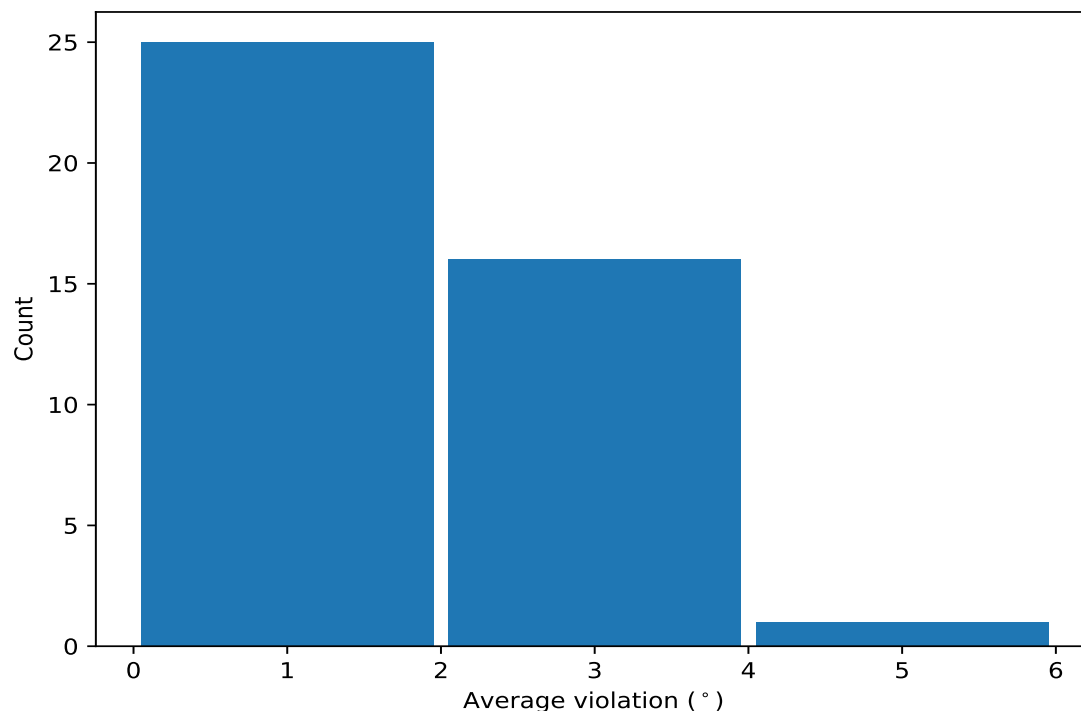


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	20	3.89	1.26	4.06
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	16	1.83	0.57	1.78
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	15	2.13	0.62	1.87
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	14	2.34	1.09	1.8
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	14	2.18	0.91	2.18
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	13	3.05	1.54	2.16
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	13	1.83	0.67	1.57
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	12	2.41	0.86	2.46
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	9	1.71	0.59	1.6
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	9	1.7	0.47	1.67
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	8	5.77	2.95	6.05
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	8	2.12	0.85	1.97
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	7	2.92	1.02	2.95
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	7	2.12	1.07	1.63
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	6	1.32	0.31	1.16
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	5	1.99	0.79	1.5
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	1.66	0.24	1.53
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	5	1.61	0.36	1.64
(1,8)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	4	2.04	0.56	2.2
(1,44)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:PHE:N	4	1.79	0.39	1.75

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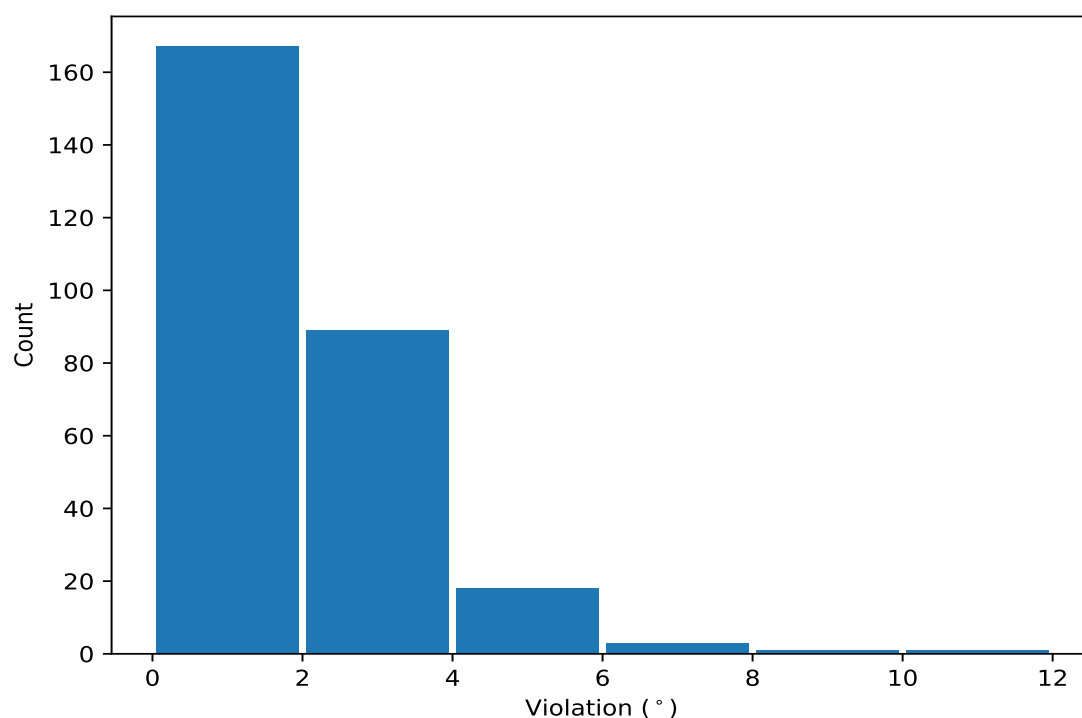
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,37)	1:60:A:THR:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	4	1.56	0.5	1.44
(1,65)	1:114:A:SER:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	4	1.43	0.33	1.3
(1,87)	1:130:A:VAL:C	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	4	1.38	0.29	1.36
(1,40)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LEU:N	4	1.3	0.26	1.24
(1,217)	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	1:50:A:GLY:N	3	3.22	0.9	3.66
(1,272)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:ALA:N	3	2.29	0.74	1.84
(1,105)	1:144:A:ASP:C	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:C	3	2.05	0.14	2.07
(1,307)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:ARG:N	3	1.95	0.56	1.67
(1,463)	1:166:A:PRO:N	1:166:A:PRO:CA	1:166:A:PRO:C	1:167:A:PRO:N	3	1.86	0.69	1.68
(1,29)	1:42:A:ASP:C	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	3	1.79	0.68	1.6
(1,257)	1:66:A:ASN:CA	1:66:A:ASN:CB	1:66:A:ASN:CG	1:66:A:ASN:OD1	3	1.37	0.11	1.37
(1,136)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ALA:N	3	1.37	0.4	1.1
(1,19)	1:33:A:ARG:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	3	1.2	0.17	1.15
(1,215)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:ALA:N	2	3.14	0.48	3.14
(1,296)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:GLN:N	2	2.49	0.47	2.49
(1,306)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:CB	1:83:A:ASP:CG	2	2.4	0.91	2.4
(1,50)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:ARG:N	2	1.78	0.37	1.78
(1,132)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:THR:N	2	1.66	0.18	1.66
(1,480)	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	1:176:A:GLU:CD	2	1.6	0.51	1.6
(1,30)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:ARG:N	2	1.56	0.06	1.56
(1,365)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ALA:N	2	1.53	0.37	1.53
(1,173)	1:30:A:PRO:C	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	2	1.36	0.04	1.36

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	20	10.17
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	9	9.31
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	5	7.17
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	16	7.01
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	8	6.59
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	6	5.89
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	12	5.59
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	16	5.29
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	15	5.25
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	12	5.09
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	20	5.0
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	1	4.73
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	16	4.69
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	1	4.64
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	2	4.57
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	3	4.56
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	11	4.48
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	8	4.47
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	19	4.39
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	17	4.39
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	13	4.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	4	4.05
(1,217)	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	1:50:A:GLY:N	9	4.03
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	18	3.96
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	11	3.92
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	5	3.85
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	11	3.75
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	7	3.74
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	19	3.71
(1,217)	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	1:50:A:GLY:N	5	3.66
(1,4)	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	1:22:A:ARG:N	3	3.66
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	10	3.65
(1,215)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:ALA:N	4	3.63
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	11	3.6
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	3	3.59
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	12	3.56
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	8	3.51
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	16	3.47
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	11	3.47
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	18	3.4
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	8	3.38
(1,272)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:ALA:N	7	3.34
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	16	3.33
(1,306)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:CB	1:83:A:ASP:CG	16	3.32
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	19	3.27
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	13	3.23
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	1	3.19
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	6	3.18
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	18	3.17
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	4	3.14
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	3	3.13
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	17	3.09
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	14	3.04
(1,296)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:GLN:N	10	2.95
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	9	2.95
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	9	2.95
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	4	2.94
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	13	2.93
(1,278)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:THR:N	17	2.92
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	10	2.91
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	5	2.89
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	19	2.87
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	7	2.86
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	8	2.83
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	4	2.82
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	6	2.82
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	10	2.82
(1,486)	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:CB	1:180:A:GLU:CG	9	2.79
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	14	2.79
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	20	2.79
(1,463)	1:166:A:PRO:N	1:166:A:PRO:CA	1:166:A:PRO:C	1:167:A:PRO:N	12	2.77
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	3	2.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	15	2.77
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	16	2.76
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	5	2.74
(1,307)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:ARG:N	10	2.73
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	10	2.72
(1,29)	1:42:A:ASP:C	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	3	2.7
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	7	2.66
(1,215)	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1:49:A:ALA:N	3	2.66
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	14	2.63
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	8	2.57
(1,8)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	7	2.57
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	6	2.55
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	11	2.53
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	14	2.53
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	18	2.53
(1,8)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	18	2.52
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	13	2.45
(1,44)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:PHE:N	9	2.37
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	1	2.35
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	9	2.31
(1,37)	1:60:A:THR:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	19	2.29
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	17	2.28
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	2	2.23
(1,52)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:HIS:N	6	2.22
(1,105)	1:144:A:ASP:C	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:C	20	2.21
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	1	2.19
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	9	2.19
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	17	2.17
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	6	2.17
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	13	2.17
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	12	2.16
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	12	2.14
(1,50)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:ARG:N	15	2.14
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	19	2.12
(1,480)	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	1:176:A:GLU:CD	10	2.11
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	4	2.07
(1,105)	1:144:A:ASP:C	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:C	14	2.07
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	14	2.04
(1,296)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:GLN:N	16	2.02
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	19	2.01
(1,65)	1:114:A:SER:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	16	1.97
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	14	1.96
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	19	1.96
(1,217)	1:49:A:ALA:N	1:49:A:ALA:CA	1:49:A:ALA:C	1:50:A:GLY:N	11	1.96
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	12	1.95
(1,136)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ALA:N	18	1.93
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	13	1.92
(1,365)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ALA:N	11	1.9
(1,105)	1:144:A:ASP:C	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:C	18	1.88
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	15	1.88
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	1	1.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	8	1.87
(1,8)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	12	1.87
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	9	1.87
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	17	1.86
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	5	1.84
(1,272)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:ALA:N	9	1.84
(1,132)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:THR:N	17	1.84
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	1.84
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	16	1.82
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	6	1.82
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	12	1.79
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	4	1.79
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	3	1.77
(1,87)	1:130:A:VAL:C	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	2	1.77
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	3	1.76
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	4	1.75
(1,44)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:PHE:N	14	1.75
(1,44)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:PHE:N	18	1.75
(1,37)	1:60:A:THR:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	3	1.75
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	10	1.74
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	17	1.74
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	8	1.73
(1,100)	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	1:143:A:LEU:N	1	1.73
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	4	1.73
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	20	1.73
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	7	1.72
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	4	1.72
(1,40)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LEU:N	2	1.71
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	8	1.71
(1,272)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:ALA:N	8	1.7
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	15	1.7
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	6	1.69
(1,463)	1:166:A:PRO:N	1:166:A:PRO:CA	1:166:A:PRO:C	1:167:A:PRO:N	13	1.68
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	18	1.68
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	20	1.68
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	12	1.68
(1,355)	1:105:A:TRP:N	1:105:A:TRP:CA	1:105:A:TRP:C	1:106:A:GLY:N	16	1.67
(1,307)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:ARG:N	3	1.67
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	3	1.67
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	2	1.67
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	8	1.66
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	16	1.65
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	14	1.64
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	18	1.63
(1,30)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:ARG:N	9	1.62
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	18	1.61
(1,225)	1:52:A:GLU:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	3	1.61
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	3	1.6
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	2	1.6
(1,185)	1:37:A:TRP:CA	1:37:A:TRP:CB	1:37:A:TRP:CG	1:37:A:TRP:CD1	2	1.6
(1,29)	1:42:A:ASP:C	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	2	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:158:A:GLY:N	1:158:A:GLY:CA	1:158:A:GLY:C	1:159:A:LYS:N	16	1.59
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	10	1.57
(1,181)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:CB	1:34:A:VAL:CG1	14	1.56
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	16	1.54
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	12	1.54
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	7	1.53
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	20	1.53
(1,87)	1:130:A:VAL:C	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	8	1.52
(1,363)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:CB	1:111:A:GLU:CG	3	1.51
(1,257)	1:66:A:ASN:CA	1:66:A:ASN:CB	1:66:A:ASN:CG	1:66:A:ASN:OD1	19	1.5
(1,30)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:ARG:N	7	1.5
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	16	1.5
(1,306)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:CB	1:83:A:ASP:CG	3	1.49
(1,132)	1:170:A:THR:N	1:170:A:THR:CA	1:170:A:THR:C	1:171:A:THR:N	10	1.49
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	20	1.46
(1,307)	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	1:84:A:ARG:N	19	1.45
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	18	1.44
(1,65)	1:114:A:SER:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	10	1.43
(1,19)	1:33:A:ARG:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	17	1.43
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	10	1.42
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	15	1.41
(1,432)	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:CB	1:145:A:VAL:CG1	9	1.41
(1,140)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:C	1:175:A:ALA:N	4	1.41
(1,50)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:ARG:N	13	1.41
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	3	1.41
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	1	1.41
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	10	1.4
(1,237)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:PRO:N	9	1.4
(1,173)	1:30:A:PRO:C	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	13	1.4
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	11	1.39
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	16	1.38
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	19	1.38
(1,257)	1:66:A:ASN:CA	1:66:A:ASN:CB	1:66:A:ASN:CG	1:66:A:ASN:OD1	15	1.37
(1,152)	1:180:A:GLU:N	1:180:A:GLU:CA	1:180:A:GLU:C	1:181:A:GLN:N	8	1.37
(1,149)	1:178:A:ASP:C	1:179:A:TYR:N	1:179:A:TYR:CA	1:179:A:TYR:C	14	1.37
(1,39)	1:61:A:PHE:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	18	1.37
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	10	1.37
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	6	1.37
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	19	1.37
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	9	1.36
(1,16)	1:32:A:GLU:N	1:32:A:GLU:CA	1:32:A:GLU:C	1:33:A:ARG:N	14	1.34
(1,122)	1:156:A:LEU:N	1:156:A:LEU:CA	1:156:A:LEU:C	1:157:A:ALA:N	15	1.33
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	7	1.33
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	13	1.33
(1,18)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:VAL:N	2	1.33
(1,40)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LEU:N	18	1.32
(1,173)	1:30:A:PRO:C	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	3	1.31
(1,114)	1:152:A:HIS:N	1:152:A:HIS:CA	1:152:A:HIS:C	1:153:A:LEU:N	15	1.31
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	8	1.3
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	2	1.3
(1,62)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	19	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,235)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:CB	1:56:A:GLN:CG	20	1.28
(1,72)	1:118:A:PHE:N	1:118:A:PHE:CA	1:118:A:PHE:C	1:119:A:GLU:N	17	1.28
(1,44)	1:64:A:HIS:N	1:64:A:HIS:CA	1:64:A:HIS:C	1:65:A:PHE:N	10	1.28
(1,104)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:VAL:N	18	1.27
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	11	1.27
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	14	1.27
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	9	1.26
(1,257)	1:66:A:ASN:CA	1:66:A:ASN:CB	1:66:A:ASN:CG	1:66:A:ASN:OD1	13	1.24
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	7	1.24
(1,169)	1:28:A:PRO:N	1:28:A:PRO:CA	1:28:A:PRO:C	1:29:A:GLY:N	8	1.21
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	20	1.21
(1,87)	1:130:A:VAL:C	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	3	1.21
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	1	1.2
(1,102)	1:143:A:LEU:N	1:143:A:LEU:CA	1:143:A:LEU:C	1:144:A:ASP:N	12	1.2
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	17	1.2
(1,8)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	14	1.19
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	6	1.18
(1,228)	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1:54:A:PRO:N	15	1.18
(1,99)	1:141:A:ALA:C	1:142:A:MET:N	1:142:A:MET:CA	1:142:A:MET:C	2	1.18
(1,65)	1:114:A:SER:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	1	1.18
(1,2)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ILE:N	11	1.17
(1,365)	1:111:A:GLU:N	1:111:A:GLU:CA	1:111:A:GLU:C	1:112:A:ALA:N	7	1.16
(1,40)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LEU:N	19	1.16
(1,19)	1:33:A:ARG:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	18	1.15
(1,92)	1:133:A:HIS:N	1:133:A:HIS:CA	1:133:A:HIS:C	1:134:A:THR:N	5	1.14
(1,65)	1:114:A:SER:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	6	1.14
(1,37)	1:60:A:THR:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	5	1.14
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	20	1.13
(1,3)	1:20:A:SER:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	7	1.13
(1,463)	1:166:A:PRO:N	1:166:A:PRO:CA	1:166:A:PRO:C	1:167:A:PRO:N	4	1.12
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	6	1.12
(1,367)	1:112:A:ALA:N	1:112:A:ALA:CA	1:112:A:ALA:C	1:113:A:PRO:N	13	1.12
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	13	1.11
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	19	1.11
(1,312)	1:85:A:PRO:N	1:85:A:PRO:CA	1:85:A:PRO:C	1:86:A:ILE:N	10	1.11
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	19	1.11
(1,136)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ALA:N	15	1.1
(1,480)	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	1:176:A:GLU:CD	12	1.09
(1,26)	1:37:A:TRP:N	1:37:A:TRP:CA	1:37:A:TRP:C	1:38:A:LEU:N	5	1.09
(1,136)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ALA:N	4	1.07
(1,118)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:VAL:N	4	1.07
(1,29)	1:42:A:ASP:C	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	7	1.07
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	3	1.06
(1,20)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:TRP:N	18	1.06
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	10	1.05
(1,37)	1:60:A:THR:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	20	1.05
(1,234)	1:55:A:ARG:C	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	10	1.03
(1,109)	1:149:A:TRP:C	1:150:A:HIS:N	1:150:A:HIS:CA	1:150:A:HIS:C	18	1.03
(1,479)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:CB	1:176:A:GLU:CG	17	1.02
(1,19)	1:33:A:ARG:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	14	1.02
(1,477)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:CB	1:174:A:GLN:CG	7	1.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,462)	1:165:A:PRO:N	1:165:A:PRO:CA	1:165:A:PRO:C	1:166:A:PRO:N	2	1.01
(1,40)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:LEU:N	8	1.01
(1,87)	1:130:A:VAL:C	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	18	1.0