Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 01:17 AM EDT

PDB ID	:	2L9W
BMRB ID	:	17490
Title	:	Solution Structure of the C-terminal domain of Prp24
Authors	:	Martin-Tumasz, S.A.; Butcher, S.E.
Deposited on	:	2011-02-25

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

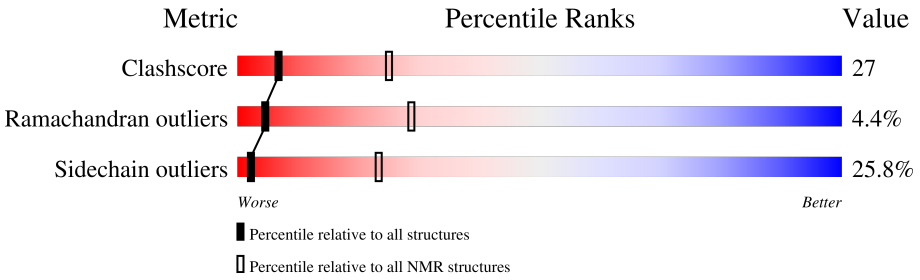
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	117	38% 43% 9% • • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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 average pairwise rmsd*.

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:294-A:399 (106)	0.68	11

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1792 atoms, of which 912 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U4/U6 snRNA-associated-splicing factor PRP24.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1792	560	912	155	160	5	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	MET	-	initiating methionine	UNP P49960
A	401	TRP	-	expression tag	UNP P49960
A	402	HIS	-	expression tag	UNP P49960
A	403	HIS	-	expression tag	UNP P49960
A	404	HIS	-	expression tag	UNP P49960
A	405	HIS	-	expression tag	UNP P49960
A	406	HIS	-	expression tag	UNP P49960
A	407	HIS	-	expression tag	UNP P49960

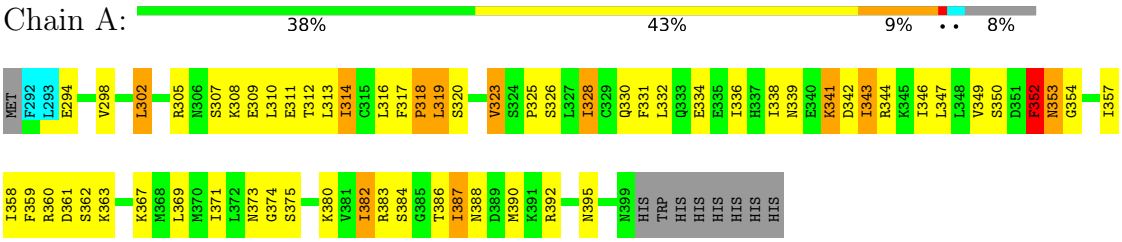
4 Residue-property plots

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: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



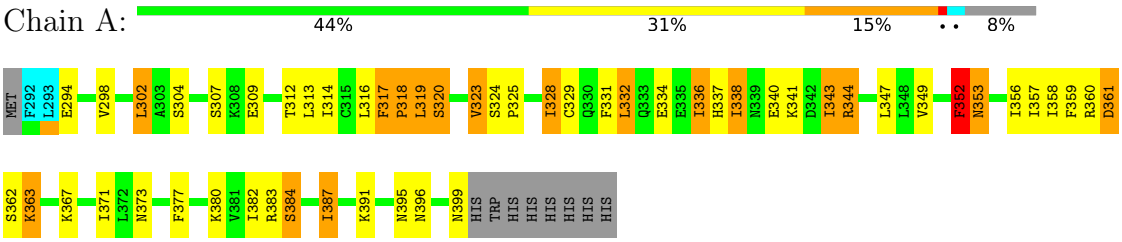
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

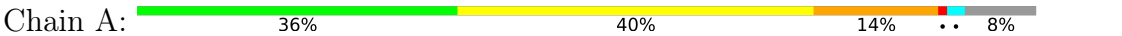
Chain A:

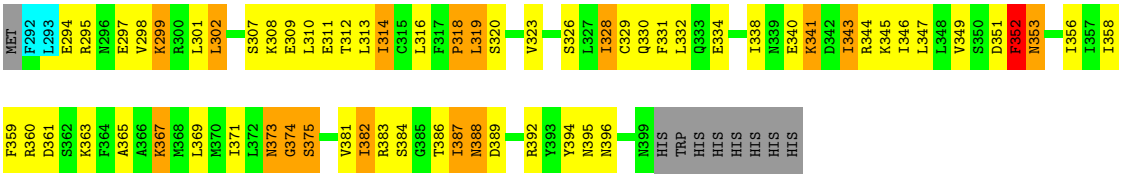


4.2.2 Score per residue for model 2

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

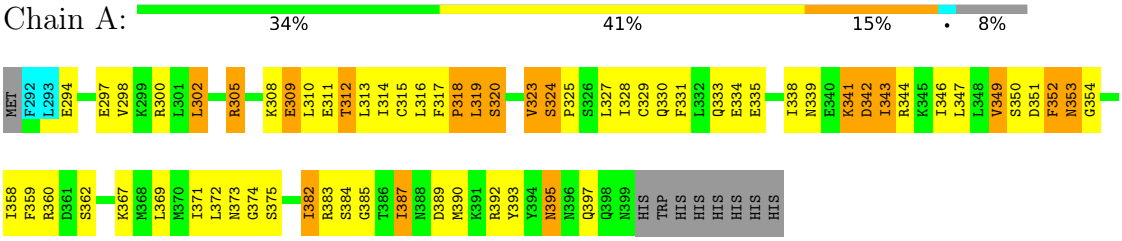
Chain A:





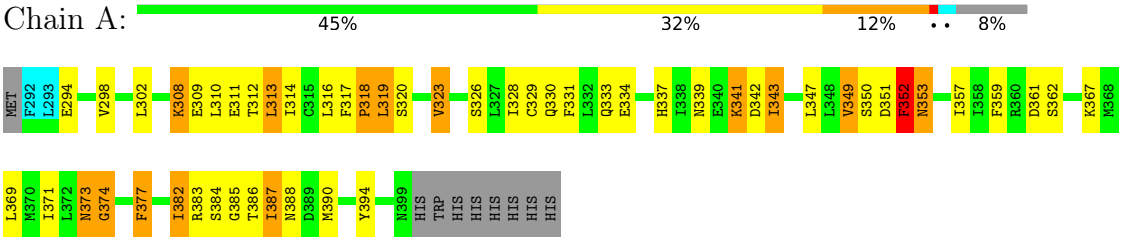
4.2.3 Score per residue for model 3

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



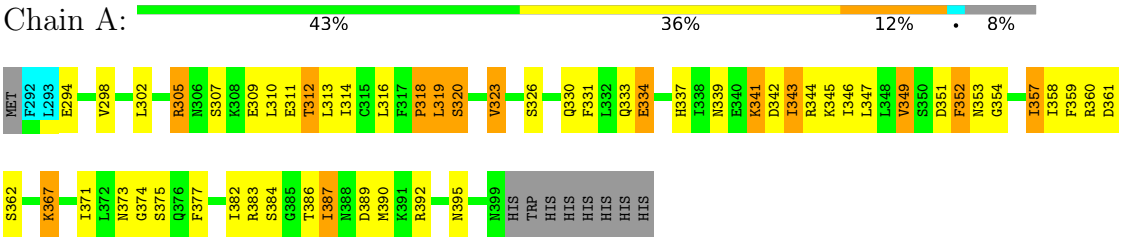
4.2.4 Score per residue for model 4

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



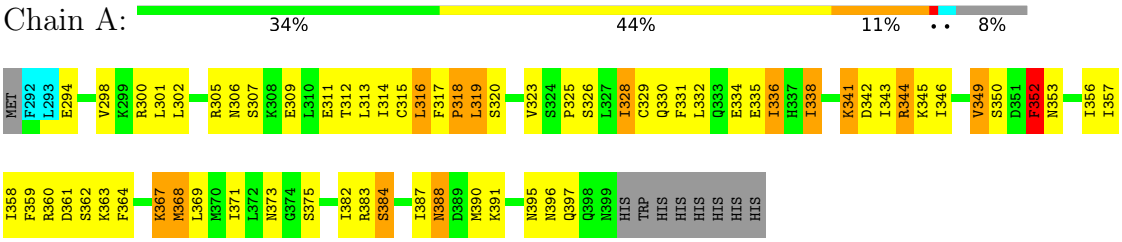
4.2.5 Score per residue for model 5

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



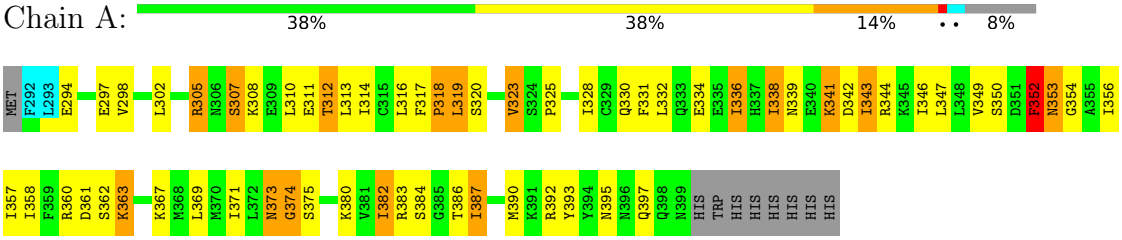
4.2.6 Score per residue for model 6

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



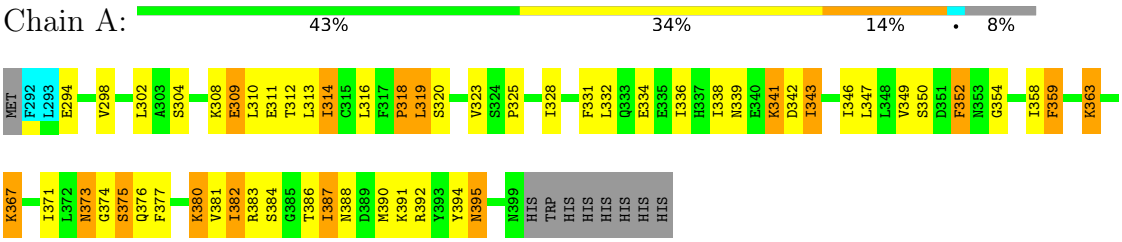
4.2.7 Score per residue for model 7

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



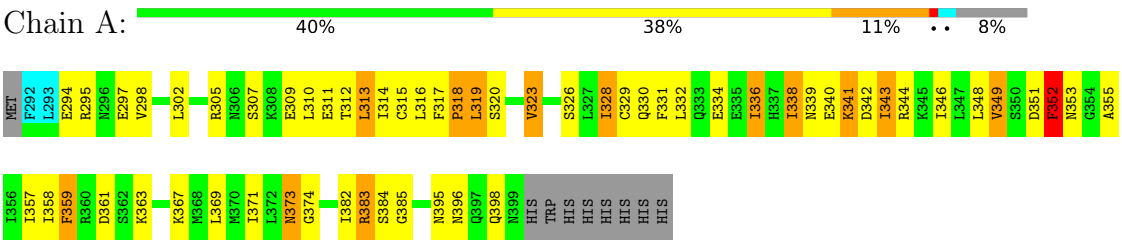
4.2.8 Score per residue for model 8

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



4.2.9 Score per residue for model 9

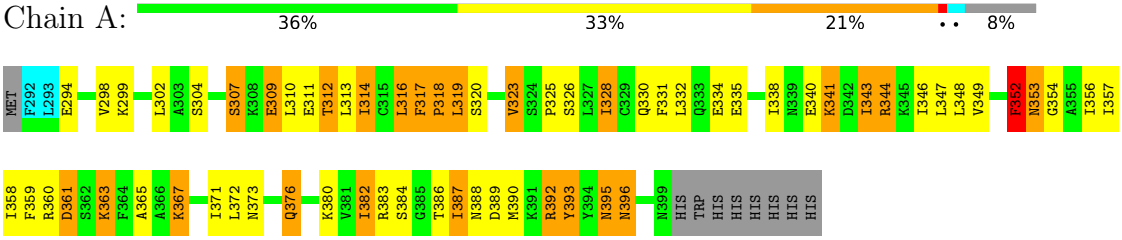
• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



4.2.10 Score per residue for model 10

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

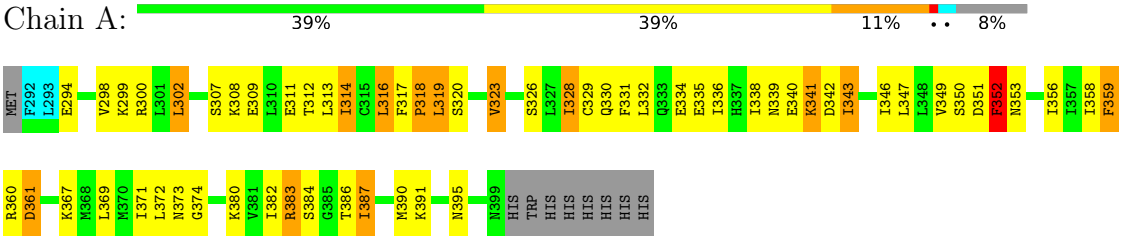
Chain A:



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

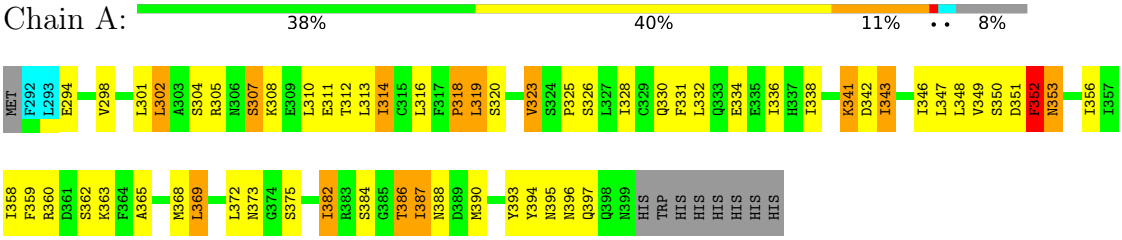
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

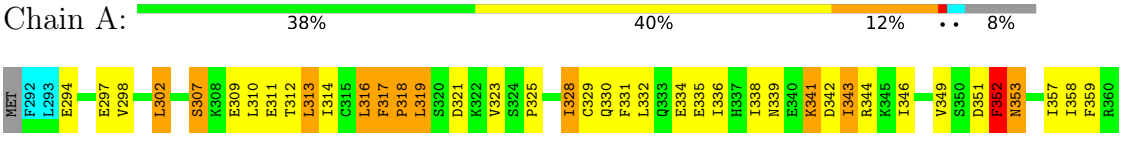
Chain A:



4.2.13 Score per residue for model 13

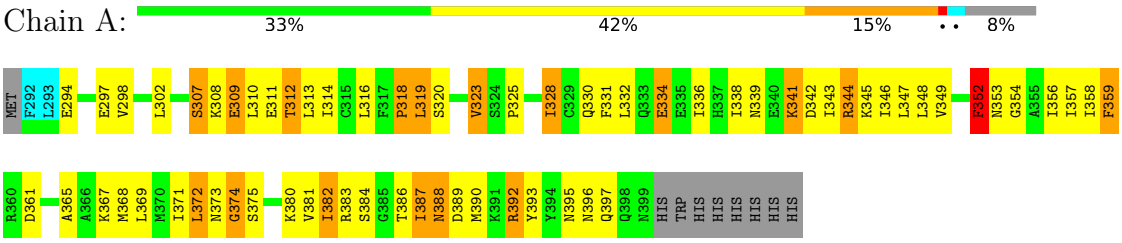
• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24

Chain A:



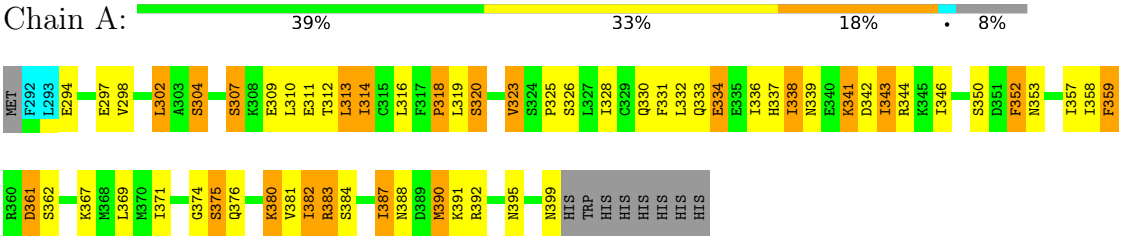
4.2.14 Score per residue for model 14

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



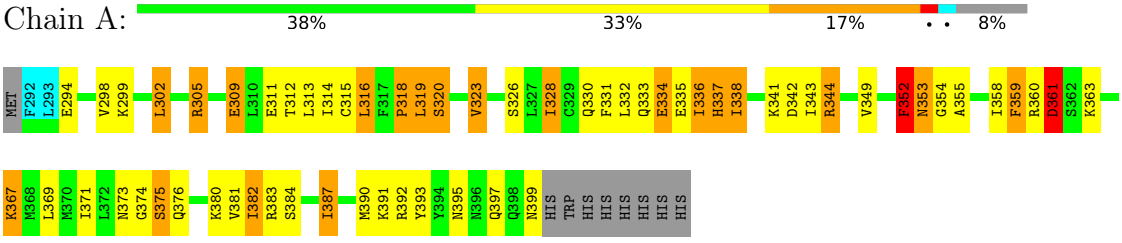
4.2.15 Score per residue for model 15

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



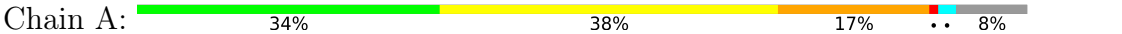
4.2.16 Score per residue for model 16

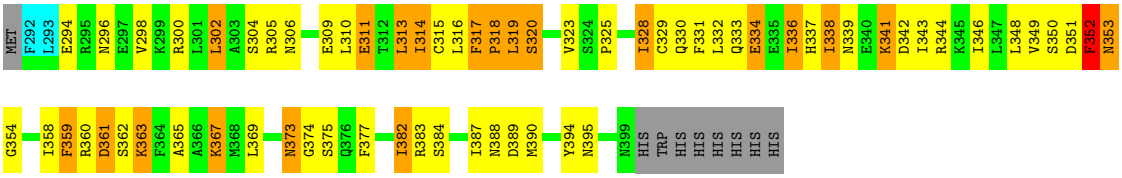
• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



4.2.17 Score per residue for model 17

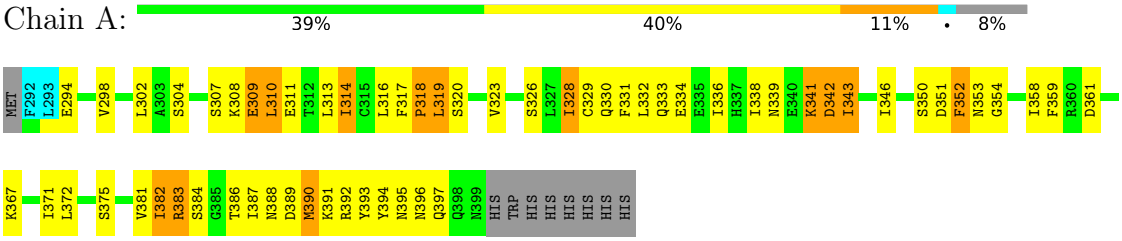
• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24





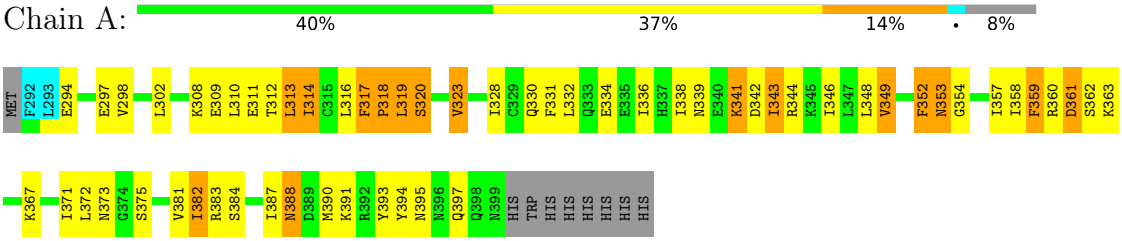
4.2.18 Score per residue for model 18

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



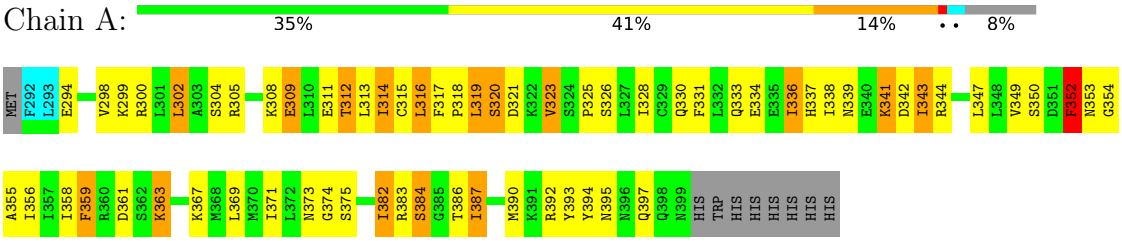
4.2.19 Score per residue for model 19

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



4.2.20 Score per residue for model 20

• Molecule 1: U4/U6 snRNA-associated-splicing factor PRP24



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
HADDOCK	refinement	2.0
UNIO	structure solution	08

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	1420
Number of shifts mapped to atoms	1415
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	861	893	893	48±5
All	All	17220	17860	17860	963

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:349:VAL:HG12	1:A:352:PHE:CE1	0.93	1.98	9	12
1:A:336:ILE:HB	1:A:338:ILE:HD13	0.83	1.48	1	4
1:A:319:LEU:HD23	1:A:328:ILE:HD12	0.82	1.50	8	4
1:A:310:LEU:HD13	1:A:387:ILE:HD11	0.81	1.53	12	3
1:A:318:PRO:HD2	1:A:319:LEU:HD23	0.81	1.53	9	7
1:A:319:LEU:HD13	1:A:353:ASN:HB3	0.80	1.50	10	3
1:A:316:LEU:HA	1:A:384:SER:OG	0.79	1.77	1	12
1:A:338:ILE:HG21	1:A:343:ILE:HD12	0.77	1.56	12	8
1:A:343:ILE:HD13	1:A:346:ILE:HB	0.76	1.56	13	11
1:A:349:VAL:HG13	1:A:352:PHE:CE1	0.76	2.16	7	4
1:A:314:ILE:HG22	1:A:386:THR:HG22	0.75	1.56	5	1
1:A:312:THR:HG22	1:A:361:ASP:HA	0.73	1.59	4	1
1:A:312:THR:HG23	1:A:361:ASP:HA	0.72	1.59	19	3
1:A:309:GLU:O	1:A:313:LEU:HG	0.72	1.84	8	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:392:ARG:HA	1:A:395:ASN:OD1	0.72	1.85	10	3
1:A:315:CYS:SG	1:A:390:MET:HB3	0.72	2.24	6	3
1:A:319:LEU:HB2	1:A:323:VAL:HG21	0.72	1.60	11	8
1:A:319:LEU:HD22	1:A:328:ILE:HD11	0.72	1.62	9	1
1:A:367:LYS:N	1:A:367:LYS:HD2	0.71	1.98	6	2
1:A:312:THR:O	1:A:358:ILE:HG23	0.71	1.85	5	2
1:A:310:LEU:HG	1:A:387:ILE:HD11	0.70	1.61	3	3
1:A:349:VAL:HG12	1:A:352:PHE:HE1	0.70	1.43	4	9
1:A:373:ASN:HB2	1:A:384:SER:OG	0.70	1.86	12	1
1:A:318:PRO:HG2	1:A:328:ILE:HD11	0.69	1.63	8	3
1:A:344:ARG:HB2	1:A:358:ILE:HG22	0.69	1.65	9	5
1:A:349:VAL:HG12	1:A:352:PHE:CD1	0.69	2.23	11	4
1:A:343:ILE:HG13	1:A:357:ILE:HG21	0.68	1.66	5	1
1:A:341:LYS:O	1:A:360:ARG:HD3	0.68	1.88	2	2
1:A:298:VAL:HG11	1:A:349:VAL:HB	0.68	1.63	17	2
1:A:313:LEU:HB3	1:A:358:ILE:CG1	0.68	2.19	12	18
1:A:319:LEU:HD22	1:A:319:LEU:N	0.66	2.05	17	2
1:A:294:GLU:O	1:A:298:VAL:HG23	0.66	1.89	8	20
1:A:319:LEU:HD12	1:A:319:LEU:H	0.66	1.49	16	1
1:A:316:LEU:HD23	1:A:357:ILE:HD13	0.66	1.67	7	2
1:A:393:TYR:O	1:A:397:GLN:HG3	0.66	1.91	18	1
1:A:373:ASN:HB3	1:A:384:SER:OG	0.65	1.91	2	5
1:A:312:THR:HG22	1:A:362:SER:N	0.65	2.06	4	1
1:A:317:PHE:CZ	1:A:393:TYR:HB3	0.65	2.26	10	1
1:A:341:LYS:O	1:A:360:ARG:HD2	0.65	1.91	3	5
1:A:308:LYS:O	1:A:311:GLU:HG2	0.65	1.92	7	11
1:A:365:ALA:O	1:A:369:LEU:HB2	0.65	1.91	12	3
1:A:339:ASN:OD1	1:A:341:LYS:HG3	0.64	1.92	18	14
1:A:316:LEU:C	1:A:318:PRO:HD3	0.64	2.13	9	19
1:A:352:PHE:O	1:A:353:ASN:HB2	0.64	1.91	13	7
1:A:373:ASN:HB3	1:A:384:SER:CB	0.64	2.22	2	6
1:A:331:PHE:HA	1:A:334:GLU:HB2	0.64	1.70	8	20
1:A:307:SER:O	1:A:311:GLU:HG2	0.63	1.92	13	6
1:A:319:LEU:HD23	1:A:353:ASN:HB3	0.63	1.68	17	1
1:A:367:LYS:O	1:A:371:ILE:HG13	0.62	1.93	1	5
1:A:367:LYS:O	1:A:371:ILE:HG12	0.62	1.93	5	13
1:A:314:ILE:HD11	1:A:359:PHE:HE1	0.62	1.55	2	7
1:A:320:SER:O	1:A:323:VAL:HG22	0.62	1.94	9	11
1:A:352:PHE:CD1	1:A:352:PHE:N	0.62	2.67	11	17
1:A:360:ARG:O	1:A:361:ASP:HB2	0.62	1.94	19	5
1:A:319:LEU:CB	1:A:323:VAL:HG21	0.62	2.25	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:ILE:O	1:A:390:MET:HG2	0.62	1.95	5	9
1:A:319:LEU:HD12	1:A:319:LEU:N	0.61	2.11	10	3
1:A:317:PHE:CZ	1:A:390:MET:HB2	0.61	2.30	7	1
1:A:298:VAL:HG11	1:A:349:VAL:HG13	0.61	1.71	4	4
1:A:343:ILE:HG22	1:A:345:LYS:N	0.60	2.11	6	2
1:A:312:THR:CG2	1:A:361:ASP:HA	0.60	2.25	4	1
1:A:311:GLU:O	1:A:362:SER:HA	0.60	1.95	19	1
1:A:301:LEU:HD13	1:A:356:ILE:HG21	0.60	1.72	2	3
1:A:344:ARG:CG	1:A:358:ILE:HB	0.60	2.26	5	1
1:A:302:LEU:HA	1:A:387:ILE:HG21	0.60	1.72	1	2
1:A:386:THR:O	1:A:390:MET:HG3	0.59	1.97	20	1
1:A:338:ILE:HG13	1:A:343:ILE:CG1	0.59	2.27	6	2
1:A:369:LEU:HG	1:A:384:SER:OG	0.59	1.97	9	3
1:A:343:ILE:HD12	1:A:357:ILE:HG23	0.59	1.73	6	1
1:A:319:LEU:HD22	1:A:319:LEU:H	0.59	1.58	17	2
1:A:328:ILE:O	1:A:332:LEU:HG	0.59	1.98	11	13
1:A:386:THR:O	1:A:390:MET:HB3	0.59	1.97	7	5
1:A:319:LEU:HD23	1:A:353:ASN:O	0.58	1.98	1	1
1:A:368:MET:O	1:A:372:LEU:HB2	0.58	1.98	12	1
1:A:347:LEU:HB2	1:A:356:ILE:CG2	0.58	2.29	20	6
1:A:314:ILE:HD11	1:A:359:PHE:CE1	0.58	2.34	2	3
1:A:317:PHE:CZ	1:A:390:MET:HA	0.58	2.33	4	1
1:A:364:PHE:O	1:A:368:MET:HB2	0.58	1.99	6	2
1:A:310:LEU:HD23	1:A:310:LEU:N	0.58	2.13	14	10
1:A:307:SER:HA	1:A:310:LEU:HD22	0.58	1.74	18	1
1:A:349:VAL:HB	1:A:354:GLY:C	0.58	2.19	14	4
1:A:314:ILE:HA	1:A:386:THR:HG22	0.57	1.77	11	5
1:A:313:LEU:HB3	1:A:358:ILE:HG13	0.57	1.76	12	13
1:A:325:PRO:O	1:A:328:ILE:HB	0.57	2.00	1	6
1:A:312:THR:HG22	1:A:358:ILE:HG23	0.57	1.76	5	6
1:A:314:ILE:HG13	1:A:369:LEU:CD2	0.56	2.30	17	3
1:A:330:GLN:O	1:A:334:GLU:HB2	0.56	2.01	16	8
1:A:338:ILE:HG23	1:A:343:ILE:HB	0.56	1.77	2	3
1:A:383:ARG:N	1:A:383:ARG:HD2	0.56	2.14	18	3
1:A:338:ILE:HG12	1:A:343:ILE:CG1	0.56	2.30	14	1
1:A:373:ASN:CB	1:A:384:SER:HB3	0.56	2.31	9	5
1:A:318:PRO:CB	1:A:382:ILE:HB	0.56	2.31	10	4
1:A:325:PRO:O	1:A:328:ILE:HG22	0.56	2.01	8	6
1:A:298:VAL:CG1	1:A:349:VAL:HG13	0.56	2.31	4	7
1:A:320:SER:H	1:A:323:VAL:CG2	0.56	2.14	15	5
1:A:312:THR:HG22	1:A:361:ASP:CA	0.55	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:343:ILE:HD12	1:A:359:PHE:HA	0.55	1.78	20	4
1:A:319:LEU:HD22	1:A:328:ILE:HG12	0.55	1.78	14	2
1:A:349:VAL:HG21	1:A:352:PHE:CE1	0.55	2.36	8	2
1:A:343:ILE:HD12	1:A:357:ILE:CG2	0.55	2.32	14	1
1:A:382:ILE:O	1:A:382:ILE:HG12	0.55	2.01	17	5
1:A:349:VAL:CG1	1:A:352:PHE:HE1	0.55	2.14	2	1
1:A:341:LYS:HE2	1:A:342:ASP:CG	0.55	2.21	4	7
1:A:336:ILE:HG21	1:A:359:PHE:HE2	0.55	1.61	9	4
1:A:317:PHE:CE1	1:A:397:GLN:HG3	0.55	2.37	13	1
1:A:311:GLU:HG3	1:A:362:SER:CB	0.54	2.33	17	2
1:A:377:PHE:HB2	1:A:382:ILE:HD12	0.54	1.80	4	1
1:A:332:LEU:O	1:A:336:ILE:HB	0.54	2.03	14	4
1:A:331:PHE:HA	1:A:334:GLU:CB	0.54	2.32	6	6
1:A:319:LEU:CD2	1:A:353:ASN:HB3	0.54	2.32	17	1
1:A:319:LEU:HD23	1:A:353:ASN:C	0.54	2.22	1	1
1:A:307:SER:O	1:A:311:GLU:HB3	0.54	2.02	2	4
1:A:319:LEU:HD12	1:A:328:ILE:CG1	0.54	2.33	17	2
1:A:376:GLN:HA	1:A:380:LYS:O	0.54	2.03	16	4
1:A:319:LEU:HD23	1:A:328:ILE:CD1	0.53	2.29	8	2
1:A:298:VAL:O	1:A:302:LEU:HD13	0.53	2.04	12	2
1:A:319:LEU:HB3	1:A:328:ILE:HD11	0.53	1.79	3	1
1:A:349:VAL:HG21	1:A:352:PHE:HE1	0.53	1.63	8	2
1:A:336:ILE:CB	1:A:338:ILE:HD13	0.53	2.27	1	2
1:A:349:VAL:HG12	1:A:354:GLY:O	0.53	2.04	17	2
1:A:343:ILE:HD13	1:A:359:PHE:HA	0.53	1.80	14	1
1:A:305:ARG:NE	1:A:305:ARG:HA	0.53	2.18	3	3
1:A:311:GLU:HG3	1:A:312:THR:N	0.53	2.17	11	4
1:A:344:ARG:HD3	1:A:358:ILE:HG22	0.52	1.81	16	4
1:A:351:ASP:HB3	1:A:352:PHE:CE1	0.52	2.39	12	4
1:A:314:ILE:HG13	1:A:369:LEU:HD23	0.52	1.80	2	3
1:A:332:LEU:HD23	1:A:336:ILE:HG13	0.52	1.80	1	1
1:A:373:ASN:CG	1:A:384:SER:HB2	0.52	2.25	6	5
1:A:373:ASN:OD1	1:A:384:SER:HB2	0.52	2.04	13	1
1:A:319:LEU:C	1:A:323:VAL:HG21	0.52	2.25	12	1
1:A:349:VAL:HG13	1:A:352:PHE:HE1	0.52	1.65	20	1
1:A:316:LEU:HD13	1:A:373:ASN:OD1	0.52	2.04	20	1
1:A:338:ILE:HG12	1:A:343:ILE:HD13	0.52	1.82	20	1
1:A:343:ILE:HG22	1:A:345:LYS:H	0.52	1.64	6	2
1:A:316:LEU:HA	1:A:384:SER:CB	0.51	2.35	16	2
1:A:349:VAL:CG1	1:A:352:PHE:CE1	0.51	2.94	5	8
1:A:352:PHE:HA	1:A:394:TYR:CD1	0.51	2.40	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:LEU:CD2	1:A:336:ILE:HG13	0.51	2.36	1	1
1:A:312:THR:HG23	1:A:361:ASP:CA	0.51	2.35	9	4
1:A:318:PRO:HD2	1:A:319:LEU:CD1	0.51	2.35	17	2
1:A:331:PHE:CA	1:A:334:GLU:HB2	0.51	2.36	8	11
1:A:394:TYR:CE1	1:A:398:GLN:HG2	0.51	2.40	13	1
1:A:299:LYS:O	1:A:302:LEU:HB2	0.51	2.04	2	3
1:A:373:ASN:CB	1:A:384:SER:CB	0.51	2.89	7	5
1:A:317:PHE:CE1	1:A:390:MET:HB2	0.51	2.41	7	1
1:A:316:LEU:HD13	1:A:384:SER:OG	0.51	2.06	13	2
1:A:319:LEU:HD11	1:A:354:GLY:N	0.51	2.21	16	1
1:A:330:GLN:O	1:A:334:GLU:HG2	0.51	2.06	13	6
1:A:315:CYS:HA	1:A:355:ALA:O	0.51	2.06	20	3
1:A:313:LEU:CB	1:A:358:ILE:HG13	0.51	2.36	13	6
1:A:332:LEU:HD11	1:A:357:ILE:HD11	0.51	1.82	1	1
1:A:333:GLN:HG2	1:A:338:ILE:O	0.51	2.06	20	2
1:A:320:SER:O	1:A:323:VAL:HG23	0.51	2.05	4	2
1:A:343:ILE:HD11	1:A:357:ILE:HG23	0.50	1.81	1	2
1:A:310:LEU:HD13	1:A:387:ILE:CD1	0.50	2.36	10	2
1:A:316:LEU:HG	1:A:373:ASN:OD1	0.50	2.06	14	2
1:A:349:VAL:HG13	1:A:352:PHE:CD1	0.50	2.40	7	3
1:A:393:TYR:HA	1:A:396:ASN:ND2	0.50	2.20	10	1
1:A:373:ASN:CB	1:A:384:SER:OG	0.50	2.59	17	7
1:A:319:LEU:HD11	1:A:353:ASN:C	0.50	2.27	3	1
1:A:333:GLN:O	1:A:337:HIS:HA	0.50	2.07	5	6
1:A:338:ILE:HG12	1:A:343:ILE:CD1	0.50	2.37	10	1
1:A:369:LEU:O	1:A:373:ASN:HB2	0.50	2.07	16	3
1:A:375:SER:HB2	1:A:382:ILE:HD11	0.50	1.84	13	1
1:A:352:PHE:CZ	1:A:354:GLY:HA3	0.49	2.42	18	1
1:A:393:TYR:O	1:A:397:GLN:HG2	0.49	2.06	14	7
1:A:313:LEU:C	1:A:313:LEU:HD12	0.49	2.28	15	6
1:A:343:ILE:CD1	1:A:359:PHE:HA	0.49	2.38	14	2
1:A:317:PHE:HB3	1:A:383:ARG:O	0.49	2.07	9	1
1:A:343:ILE:CD1	1:A:346:ILE:HB	0.49	2.38	17	4
1:A:352:PHE:HB3	1:A:394:TYR:CG	0.49	2.43	20	4
1:A:358:ILE:HG22	1:A:359:PHE:O	0.49	2.07	3	1
1:A:344:ARG:HB2	1:A:358:ILE:CG2	0.49	2.37	6	2
1:A:313:LEU:HD23	1:A:358:ILE:CG1	0.49	2.37	11	4
1:A:317:PHE:N	1:A:318:PRO:HD3	0.49	2.23	18	7
1:A:346:ILE:HA	1:A:357:ILE:HG23	0.49	1.83	5	1
1:A:332:LEU:O	1:A:336:ILE:HG12	0.49	2.08	7	1
1:A:316:LEU:HD12	1:A:318:PRO:HG3	0.49	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:LEU:HD22	1:A:387:ILE:HG23	0.49	1.85	20	1
1:A:319:LEU:CD2	1:A:328:ILE:HD12	0.48	2.38	12	3
1:A:320:SER:H	1:A:323:VAL:HG23	0.48	1.67	1	4
1:A:373:ASN:HB3	1:A:384:SER:HB3	0.48	1.85	17	3
1:A:328:ILE:HG22	1:A:329:CYS:N	0.48	2.23	11	8
1:A:329:CYS:O	1:A:333:GLN:HG3	0.48	2.08	18	2
1:A:318:PRO:HB3	1:A:382:ILE:HB	0.48	1.85	10	9
1:A:316:LEU:HD12	1:A:373:ASN:OD1	0.48	2.08	5	2
1:A:373:ASN:HB3	1:A:384:SER:N	0.48	2.24	11	2
1:A:311:GLU:HB3	1:A:362:SER:CB	0.48	2.39	15	1
1:A:331:PHE:HA	1:A:334:GLU:CG	0.47	2.38	4	1
1:A:373:ASN:OD1	1:A:384:SER:HB3	0.47	2.09	12	2
1:A:387:ILE:O	1:A:391:LYS:HG2	0.47	2.08	16	4
1:A:313:LEU:HB3	1:A:358:ILE:HG12	0.47	1.85	2	3
1:A:369:LEU:HD11	1:A:385:GLY:HA2	0.47	1.85	4	3
1:A:373:ASN:ND2	1:A:384:SER:HB2	0.47	2.25	6	4
1:A:352:PHE:HB3	1:A:394:TYR:HB2	0.47	1.85	4	1
1:A:306:ASN:O	1:A:309:GLU:HG2	0.47	2.10	17	1
1:A:390:MET:HG3	1:A:391:LYS:N	0.47	2.23	15	4
1:A:349:VAL:CG1	1:A:352:PHE:CD1	0.47	2.98	10	2
1:A:318:PRO:HD2	1:A:319:LEU:CD2	0.47	2.36	18	2
1:A:310:LEU:HD13	1:A:310:LEU:N	0.47	2.24	18	1
1:A:347:LEU:HB2	1:A:356:ILE:HG23	0.47	1.86	20	1
1:A:363:LYS:O	1:A:367:LYS:HB2	0.47	2.09	16	3
1:A:349:VAL:HG23	1:A:354:GLY:C	0.47	2.30	19	3
1:A:375:SER:O	1:A:381:VAL:HA	0.47	2.10	18	6
1:A:319:LEU:CA	1:A:323:VAL:HG21	0.47	2.40	12	1
1:A:320:SER:H	1:A:323:VAL:HG21	0.47	1.70	16	1
1:A:343:ILE:HD11	1:A:357:ILE:CG2	0.46	2.41	1	1
1:A:306:ASN:O	1:A:309:GLU:HB2	0.46	2.10	6	1
1:A:338:ILE:CG2	1:A:343:ILE:HD12	0.46	2.41	7	3
1:A:316:LEU:HA	1:A:384:SER:HG	0.46	1.68	19	2
1:A:312:THR:HG21	1:A:344:ARG:HH11	0.46	1.70	7	1
1:A:336:ILE:HG12	1:A:372:LEU:HD11	0.46	1.87	14	1
1:A:387:ILE:HG13	1:A:388:ASN:N	0.46	2.25	19	3
1:A:343:ILE:HG13	1:A:357:ILE:HG23	0.46	1.88	10	1
1:A:338:ILE:CG2	1:A:343:ILE:HG12	0.46	2.41	3	1
1:A:319:LEU:HD13	1:A:353:ASN:CB	0.46	2.41	16	1
1:A:394:TYR:O	1:A:397:GLN:HB2	0.45	2.12	12	1
1:A:338:ILE:HG13	1:A:343:ILE:HG12	0.45	1.87	1	1
1:A:336:ILE:HB	1:A:338:ILE:HD12	0.45	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:THR:O	1:A:358:ILE:HA	0.45	2.10	15	2
1:A:308:LYS:HA	1:A:311:GLU:OE2	0.45	2.11	18	1
1:A:315:CYS:HB3	1:A:390:MET:SD	0.45	2.52	20	1
1:A:388:ASN:O	1:A:392:ARG:HD2	0.45	2.11	14	1
1:A:351:ASP:C	1:A:352:PHE:CG	0.45	2.90	11	2
1:A:325:PRO:HB3	1:A:348:LEU:HD22	0.45	1.89	12	1
1:A:394:TYR:HA	1:A:397:GLN:HG3	0.45	1.89	18	1
1:A:311:GLU:HG3	1:A:362:SER:HB2	0.45	1.89	17	1
1:A:331:PHE:CE1	1:A:335:GLU:HG3	0.44	2.46	11	4
1:A:393:TYR:C	1:A:397:GLN:HG3	0.44	2.32	18	1
1:A:338:ILE:HG13	1:A:343:ILE:CD1	0.44	2.42	1	1
1:A:314:ILE:HD13	1:A:369:LEU:HB2	0.44	1.90	9	1
1:A:330:GLN:O	1:A:334:GLU:N	0.44	2.51	15	9
1:A:320:SER:N	1:A:323:VAL:HG21	0.44	2.27	4	1
1:A:312:THR:HA	1:A:362:SER:CA	0.44	2.42	3	2
1:A:351:ASP:HB3	1:A:352:PHE:CZ	0.44	2.48	9	2
1:A:311:GLU:C	1:A:313:LEU:H	0.44	2.16	6	1
1:A:312:THR:O	1:A:365:ALA:HB2	0.44	2.11	14	2
1:A:361:ASP:OD2	1:A:363:LYS:HB2	0.44	2.12	20	3
1:A:313:LEU:HA	1:A:357:ILE:O	0.44	2.12	13	2
1:A:313:LEU:HD23	1:A:358:ILE:HG13	0.44	1.89	16	1
1:A:319:LEU:HG	1:A:328:ILE:CD1	0.44	2.43	16	1
1:A:311:GLU:HG3	1:A:362:SER:HB3	0.44	1.89	7	1
1:A:360:ARG:O	1:A:361:ASP:HB3	0.43	2.12	16	1
1:A:314:ILE:HG21	1:A:369:LEU:HD12	0.43	1.89	15	1
1:A:349:VAL:O	1:A:349:VAL:HG12	0.43	2.14	7	1
1:A:315:CYS:SG	1:A:315:CYS:O	0.43	2.76	6	2
1:A:324:SER:O	1:A:327:LEU:HB2	0.43	2.13	3	1
1:A:342:ASP:O	1:A:360:ARG:HG3	0.43	2.13	3	1
1:A:319:LEU:HD22	1:A:328:ILE:HG13	0.43	1.90	19	1
1:A:374:GLY:N	1:A:382:ILE:O	0.43	2.52	14	5
1:A:336:ILE:HD12	1:A:372:LEU:HD11	0.43	1.89	18	1
1:A:332:LEU:CD2	1:A:338:ILE:HG12	0.43	2.43	1	1
1:A:310:LEU:HA	1:A:313:LEU:HG	0.43	1.90	19	6
1:A:312:THR:HG22	1:A:362:SER:H	0.43	1.72	4	1
1:A:318:PRO:CD	1:A:319:LEU:HD23	0.43	2.36	9	1
1:A:313:LEU:HB2	1:A:358:ILE:HG13	0.43	1.91	13	1
1:A:320:SER:O	1:A:323:VAL:CG2	0.43	2.67	7	2
1:A:319:LEU:HD12	1:A:328:ILE:HG12	0.43	1.91	17	1
1:A:369:LEU:HD11	1:A:385:GLY:CA	0.42	2.44	4	1
1:A:368:MET:O	1:A:372:LEU:N	0.42	2.52	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:310:LEU:HD13	1:A:387:ILE:CG1	0.42	2.44	15	1
1:A:312:THR:HA	1:A:362:SER:HA	0.42	1.92	5	3
1:A:338:ILE:HG12	1:A:343:ILE:HD11	0.42	1.90	14	1
1:A:300:ARG:O	1:A:304:SER:HB2	0.42	2.13	17	1
1:A:343:ILE:HD11	1:A:357:ILE:HG12	0.42	1.91	19	1
1:A:319:LEU:HB3	1:A:323:VAL:HG21	0.42	1.92	19	1
1:A:325:PRO:HA	1:A:328:ILE:HD12	0.42	1.91	1	1
1:A:343:ILE:HD12	1:A:343:ILE:HA	0.42	1.65	1	2
1:A:341:LYS:HE3	1:A:342:ASP:CG	0.42	2.34	19	1
1:A:331:PHE:CE2	1:A:335:GLU:HG3	0.42	2.49	10	1
1:A:310:LEU:N	1:A:310:LEU:CD2	0.42	2.81	14	2
1:A:382:ILE:H	1:A:382:ILE:HD13	0.42	1.73	15	1
1:A:302:LEU:HD11	1:A:352:PHE:CZ	0.42	2.50	17	1
1:A:336:ILE:HB	1:A:338:ILE:HG23	0.42	1.92	17	1
1:A:338:ILE:HG23	1:A:343:ILE:HG12	0.42	1.90	3	1
1:A:320:SER:N	1:A:323:VAL:CG2	0.42	2.83	4	1
1:A:387:ILE:N	1:A:387:ILE:HD13	0.42	2.29	10	1
1:A:302:LEU:HD22	1:A:387:ILE:HG22	0.42	1.91	13	1
1:A:316:LEU:HA	1:A:384:SER:HB3	0.42	1.92	13	1
1:A:345:LYS:O	1:A:357:ILE:HG23	0.42	2.15	5	1
1:A:305:ARG:HA	1:A:305:ARG:CZ	0.42	2.44	7	1
1:A:361:ASP:OD1	1:A:363:LYS:HE3	0.42	2.14	7	1
1:A:294:GLU:HG3	1:A:295:ARG:H	0.42	1.74	9	1
1:A:375:SER:O	1:A:381:VAL:HG13	0.41	2.15	2	2
1:A:311:GLU:HB3	1:A:362:SER:HB2	0.41	1.91	15	2
1:A:363:LYS:HD2	1:A:363:LYS:N	0.41	2.30	8	1
1:A:317:PHE:CZ	1:A:397:GLN:HG3	0.41	2.50	13	1
1:A:383:ARG:C	1:A:384:SER:HG	0.41	2.18	13	1
1:A:349:VAL:HB	1:A:354:GLY:O	0.41	2.16	20	1
1:A:316:LEU:O	1:A:354:GLY:CA	0.41	2.68	19	1
1:A:338:ILE:HD13	1:A:338:ILE:H	0.41	1.76	15	1
1:A:319:LEU:HD22	1:A:328:ILE:CG1	0.41	2.46	18	1
1:A:316:LEU:O	1:A:318:PRO:HD3	0.41	2.16	20	1
1:A:324:SER:HB3	1:A:325:PRO:HD2	0.41	1.92	1	1
1:A:336:ILE:HD12	1:A:372:LEU:HD13	0.41	1.91	13	1
1:A:352:PHE:HA	1:A:394:TYR:CE1	0.41	2.51	13	1
1:A:338:ILE:HG21	1:A:359:PHE:CD2	0.41	2.51	15	1
1:A:305:ARG:HD2	1:A:305:ARG:O	0.41	2.16	5	1
1:A:312:THR:O	1:A:312:THR:HG22	0.41	2.16	15	2
1:A:388:ASN:O	1:A:392:ARG:HG2	0.40	2.16	2	1
1:A:319:LEU:CD1	1:A:353:ASN:HB3	0.40	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:328:ILE:CG2	1:A:348:LEU:HD11	0.40	2.46	17	1
1:A:352:PHE:CE1	1:A:354:GLY:HA3	0.40	2.51	18	1
1:A:386:THR:N	1:A:389:ASP:HB2	0.40	2.31	5	1
1:A:349:VAL:O	1:A:354:GLY:N	0.40	2.55	10	1
1:A:342:ASP:HA	1:A:360:ARG:HE	0.40	1.76	17	1
1:A:349:VAL:HG11	1:A:390:MET:SD	0.40	2.56	20	1
1:A:317:PHE:HZ	1:A:397:GLN:CG	0.40	2.28	6	1
1:A:338:ILE:HG13	1:A:343:ILE:HD11	0.40	1.93	6	1
1:A:344:ARG:HD3	1:A:358:ILE:CG2	0.40	2.46	10	1
1:A:314:ILE:HA	1:A:386:THR:CG2	0.40	2.46	12	1
1:A:319:LEU:N	1:A:319:LEU:HD13	0.40	2.32	1	1
1:A:391:LYS:O	1:A:394:TYR:HB3	0.40	2.17	13	1
1:A:319:LEU:N	1:A:319:LEU:CD2	0.40	2.76	17	1
1:A:317:PHE:CD2	1:A:393:TYR:HB3	0.40	2.52	19	1
1:A:338:ILE:HG21	1:A:343:ILE:HG12	0.40	1.93	20	1
1:A:338:ILE:HG13	1:A:343:ILE:HG13	0.40	1.94	7	1
1:A:308:LYS:HA	1:A:311:GLU:OE1	0.40	2.17	8	1
1:A:316:LEU:HG	1:A:373:ASN:CG	0.40	2.36	17	1
1:A:344:ARG:HB2	1:A:358:ILE:O	0.40	2.16	17	1
1:A:369:LEU:HD21	1:A:384:SER:HB2	0.40	1.91	17	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/117 (90%)	91±2 (86±2%)	10±2 (9±2%)	5±1 (4±1%)	4	29
All	All	2100/2340 (90%)	1814 (86%)	194 (9%)	92 (4%)	4	29

All 11 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	318	PRO	19
1	A	353	ASN	18

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Mol	Chain	Res	Type	Models (Total)
1	A	352	PHE	15
1	A	359	PHE	13
1	A	374	GLY	12
1	A	361	ASP	5
1	A	320	SER	3
1	A	304	SER	3
1	A	312	THR	2
1	A	360	ARG	1
1	A	351	ASP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	98/109 (90%)	73±4 (74±4%)	25±4 (26±4%)	2 23
All	All	1960/2180 (90%)	1454 (74%)	506 (26%)	2 23

All 73 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	302	LEU	20
1	A	319	LEU	19
1	A	352	PHE	19
1	A	383	ARG	19
1	A	395	ASN	19
1	A	341	LYS	19
1	A	382	ILE	19
1	A	314	ILE	18
1	A	343	ILE	17
1	A	323	VAL	16
1	A	387	ILE	15
1	A	328	ILE	12
1	A	309	GLU	12
1	A	326	SER	12
1	A	375	SER	12
1	A	388	ASN	11

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Mol	Chain	Res	Type	Models (Total)
1	A	350	SER	11
1	A	363	LYS	10
1	A	342	ASP	10
1	A	305	ARG	9
1	A	307	SER	8
1	A	336	ILE	8
1	A	396	ASN	8
1	A	297	GLU	8
1	A	392	ARG	8
1	A	317	PHE	7
1	A	320	SER	7
1	A	338	ILE	7
1	A	344	ARG	7
1	A	380	LYS	7
1	A	367	LYS	7
1	A	389	ASP	7
1	A	361	ASP	6
1	A	312	THR	6
1	A	347	LEU	6
1	A	373	ASN	6
1	A	349	VAL	6
1	A	313	LEU	6
1	A	316	LEU	6
1	A	304	SER	5
1	A	340	GLU	5
1	A	377	PHE	5
1	A	372	LEU	5
1	A	334	GLU	5
1	A	300	ARG	4
1	A	346	ILE	4
1	A	348	LEU	4
1	A	384	SER	3
1	A	399	ASN	3
1	A	299	LYS	3
1	A	351	ASP	3
1	A	369	LEU	3
1	A	337	HIS	2
1	A	321	ASP	2
1	A	390	MET	2
1	A	329	CYS	1
1	A	332	LEU	1
1	A	295	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	345	LYS	1
1	A	324	SER	1
1	A	308	LYS	1
1	A	357	ILE	1
1	A	368	MET	1
1	A	391	LYS	1
1	A	398	GLN	1
1	A	376	GLN	1
1	A	393	TYR	1
1	A	386	THR	1
1	A	335	GLU	1
1	A	296	ASN	1
1	A	311	GLU	1
1	A	310	LEU	1
1	A	353	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1420
Number of shifts mapped to atoms	1415
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 5 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	400	HIS	H	7.961	0.008	1
1	A	400	HIS	CA	60.813	0	1
1	A	400	HIS	N	118.498	0.223	1
1	A	401	TRP	HE1	10.059	0.009	.
1	A	401	TRP	NE1	129.233	0.071	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	109	-0.23 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	104	-0.01 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	105	0.00 ± 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	106	0.93 ± 0.38	Should be applied

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. 1383 atoms were assigned a chemical shift out of a possible 1538. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	527/530 (99%)	214/214 (100%)	209/212 (99%)	104/104 (100%)
Sidechain	802/923 (87%)	545/596 (91%)	243/282 (86%)	14/45 (31%)
Aromatic	54/85 (64%)	28/42 (67%)	26/42 (62%)	0/1 (0%)
Overall	1383/1538 (90%)	787/852 (92%)	478/536 (89%)	118/150 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1415 atoms were assigned a chemical shift out of a possible 1574. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	535/540 (99%)	217/218 (100%)	213/216 (99%)	105/106 (99%)
Sidechain	818/939 (87%)	556/607 (92%)	248/287 (86%)	14/45 (31%)
Aromatic	62/95 (65%)	32/47 (68%)	30/47 (64%)	0/1 (0%)
Overall	1415/1574 (90%)	805/872 (92%)	491/550 (89%)	119/152 (78%)

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.

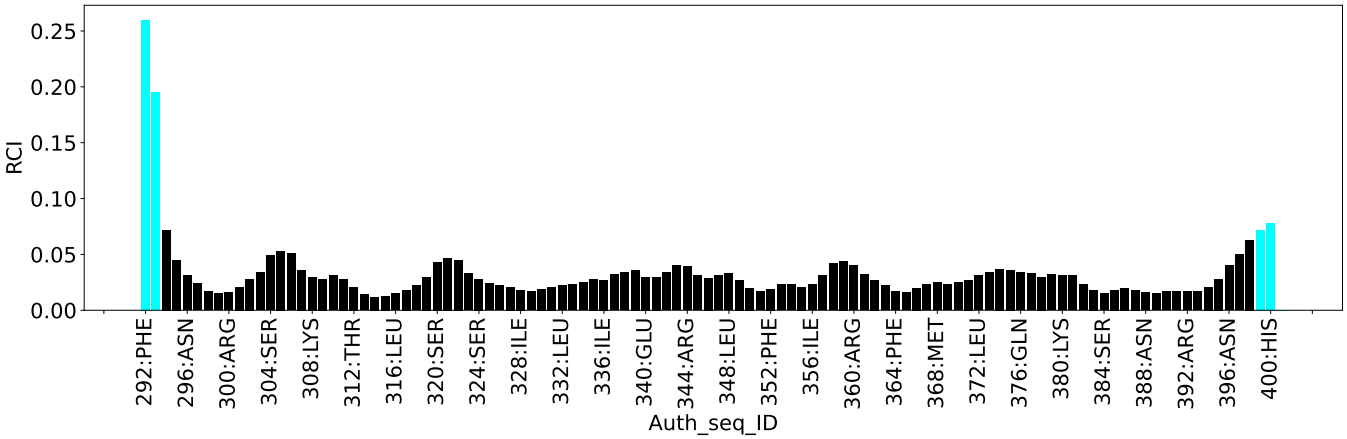
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	391	LYS	HG2	-0.29	0.13 – 2.61	-6.7
1	A	391	LYS	HG3	-0.29	0.04 – 2.67	-6.3
1	A	378	GLN	HG3	0.81	0.91 – 3.68	-5.3

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	917
Intra-residue (|i-j|=0)	282
Sequential (|i-j|=1)	138
Medium range (|i-j|>1 and |i-j|<5)	201
Long range (|i-j|≥5)	243
Inter-chain	0
Hydrogen bond restraints	53
Disulfide bond restraints	0
Total dihedral-angle restraints	177
Number of unmapped restraints	0
Number of restraints per residue	9.4
Number of long range restraints per residue[1]	2.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	7.5	0.2
0.2-0.5 (Medium)	1.2	0.37
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	17.4	9.4
10.0-20.0 (Medium)	0.3	16.2
>20.0 (Large)	None	None

9 Distance violation analysis (i)

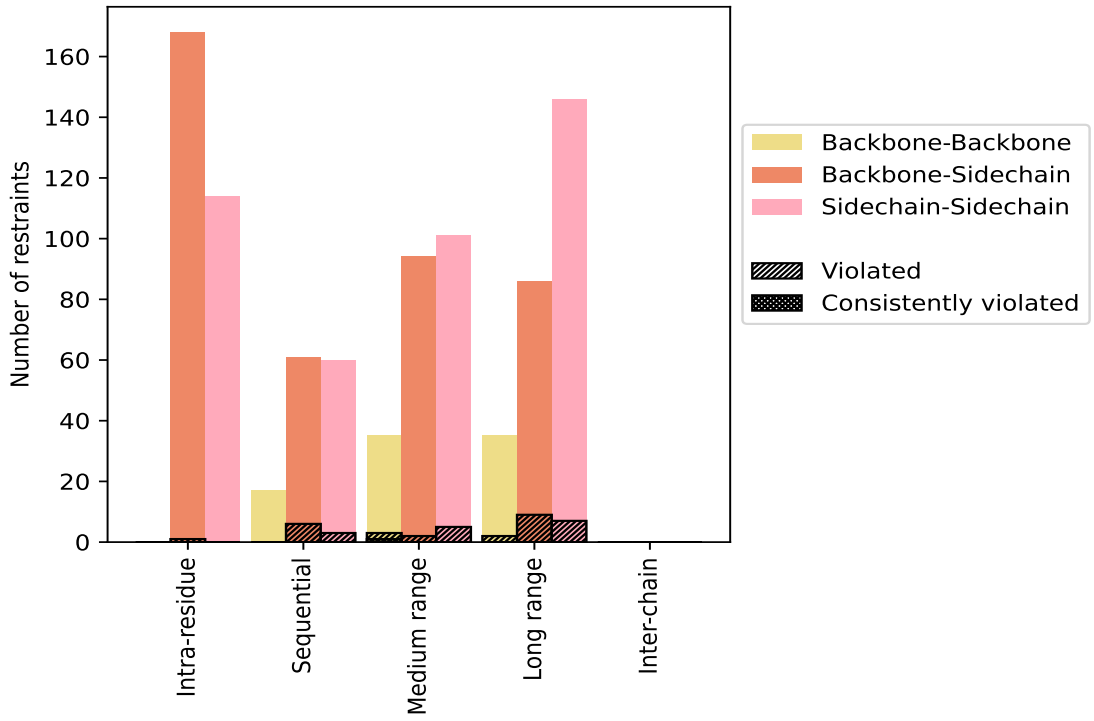
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	282	30.8	1	0.4	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	168	18.3	1	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	114	12.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	138	15.0	9	6.5	1.0	0	0.0	0.0
Backbone-Backbone	17	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	6.7	6	9.8	0.7	0	0.0	0.0
Sidechain-Sidechain	60	6.5	3	5.0	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	201	21.9	8	4.0	0.9	1	0.5	0.1
Backbone-Backbone	6	0.7	1	16.7	0.1	1	16.7	0.1
Backbone-Sidechain	94	10.3	2	2.1	0.2	0	0.0	0.0
Sidechain-Sidechain	101	11.0	5	5.0	0.5	0	0.0	0.0
Long range (|i-j|≥5)	243	26.5	16	6.6	1.7	0	0.0	0.0
Backbone-Backbone	11	1.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	86	9.4	9	10.5	1.0	0	0.0	0.0
Sidechain-Sidechain	146	15.9	7	4.8	0.8	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	53	5.8	4	7.5	0.4	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	917	100.0	38	4.1	4.1	1	0.1	0.1
Backbone-Backbone	87	9.5	5	5.7	0.5	1	1.1	0.1
Backbone-Sidechain	409	44.6	18	4.4	2.0	0	0.0	0.0
Sidechain-Sidechain	421	45.9	15	3.6	1.6	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



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	3	3	0	6	0.15	0.23	0.04	0.14
2	0	5	2	7	0	14	0.15	0.35	0.07	0.12
3	0	1	1	5	0	7	0.14	0.2	0.03	0.13
4	0	2	2	6	0	10	0.18	0.33	0.06	0.16
5	0	2	2	5	0	9	0.14	0.21	0.03	0.14
6	0	1	1	2	0	4	0.15	0.19	0.03	0.14
7	1	2	3	3	0	9	0.17	0.34	0.07	0.14
8	1	2	2	6	0	11	0.14	0.2	0.02	0.13
9	0	4	2	3	0	9	0.17	0.31	0.07	0.13
10	0	1	3	5	0	9	0.14	0.2	0.03	0.14
11	0	1	1	2	0	4	0.16	0.24	0.05	0.13

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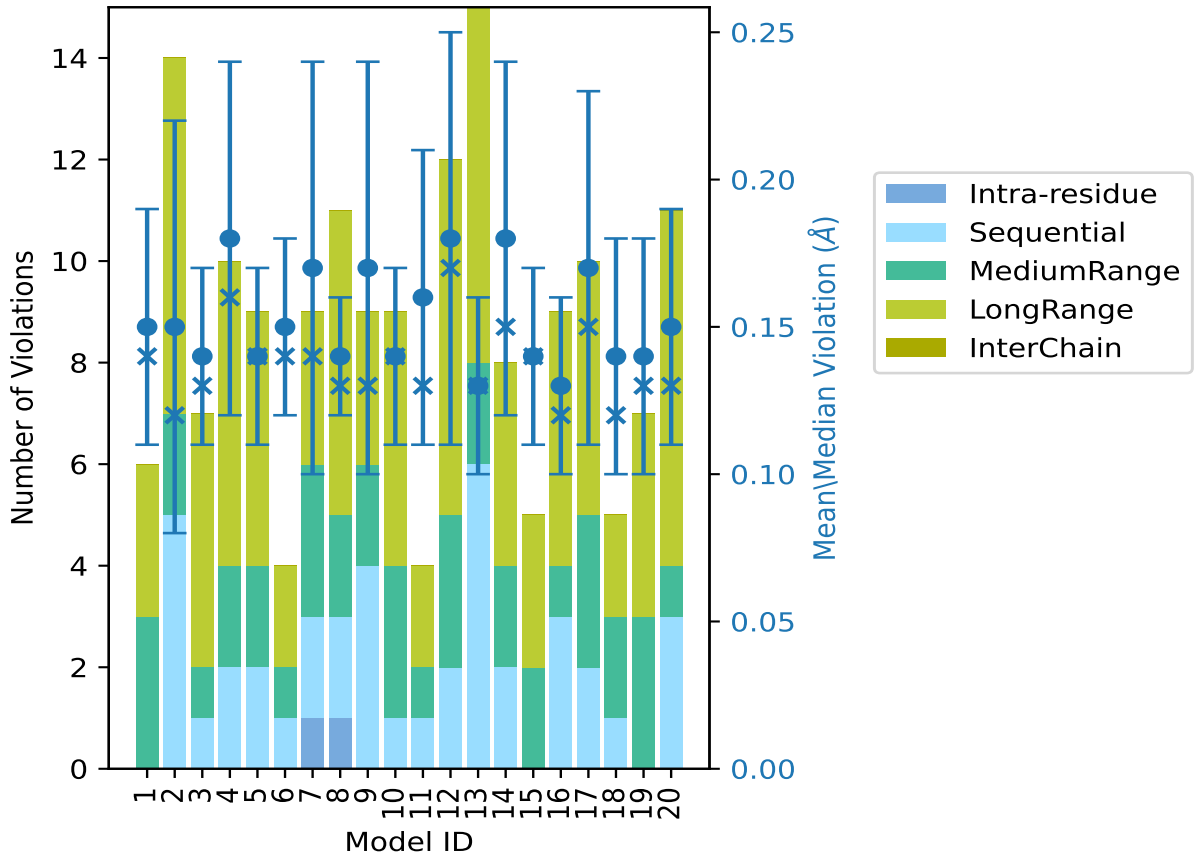
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	3	7	0	12	0.18	0.37	0.07	0.17
13	0	6	2	7	0	15	0.13	0.23	0.03	0.13
14	0	2	2	4	0	8	0.18	0.33	0.06	0.15
15	0	0	2	3	0	5	0.14	0.18	0.03	0.14
16	0	3	1	5	0	9	0.13	0.19	0.03	0.12
17	0	2	3	5	0	10	0.17	0.3	0.06	0.15
18	0	1	2	2	0	5	0.14	0.22	0.04	0.12
19	0	0	3	4	0	7	0.14	0.24	0.04	0.13
20	0	3	1	7	0	11	0.15	0.22	0.04	0.13

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

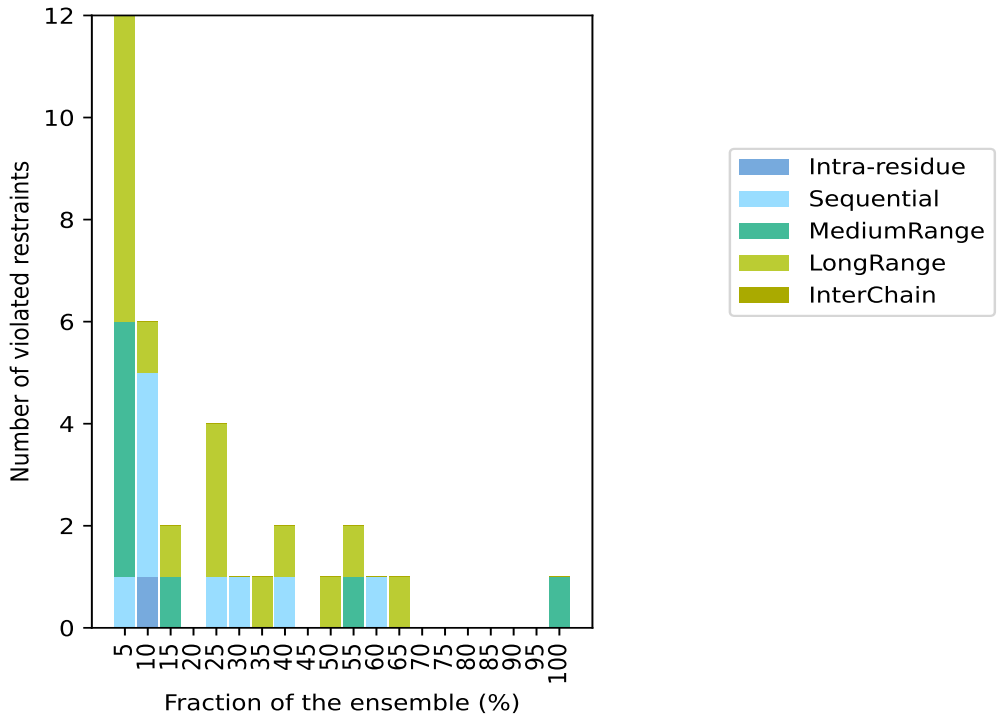
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 830(IR:281, SQ:129, MR:193, LR:227, 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]	%
0	1	5	6	0	12	1	5.0
1	4	0	1	0	6	2	10.0
0	0	1	1	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	1	0	3	0	4	5	25.0
0	1	0	0	0	1	6	30.0
0	0	0	1	0	1	7	35.0
0	1	0	1	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	1	1	0	2	11	55.0
0	1	0	0	0	1	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	1	0	0	1	20	100.0

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

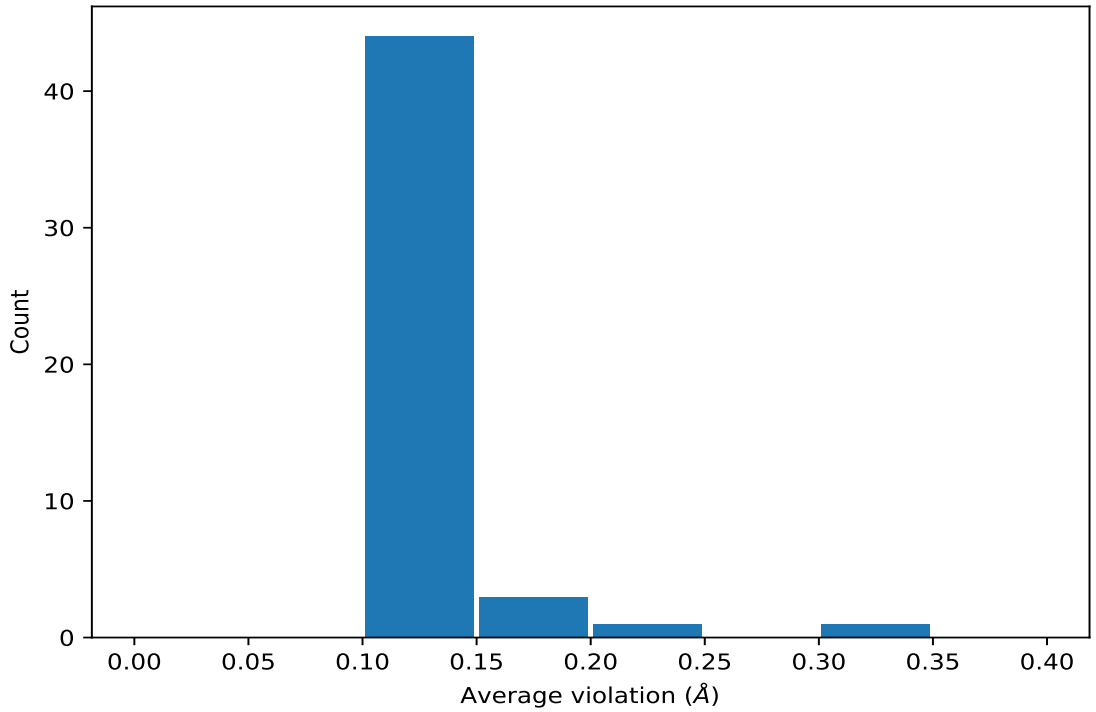
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the 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)
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	20	0.21	0.02	0.21
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	13	0.15	0.03	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	13	0.15	0.03	0.15
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	12	0.13	0.01	0.13
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	12	0.12	0.01	0.12
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	12	0.12	0.01	0.12
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	11	0.15	0.02	0.15
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	11	0.15	0.02	0.15
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	11	0.15	0.02	0.15
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	11	0.13	0.01	0.13
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	11	0.13	0.01	0.13
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	11	0.13	0.01	0.13
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	10	0.13	0.01	0.13
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	8	0.32	0.04	0.33
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	8	0.19	0.03	0.2
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	7	0.15	0.03	0.15

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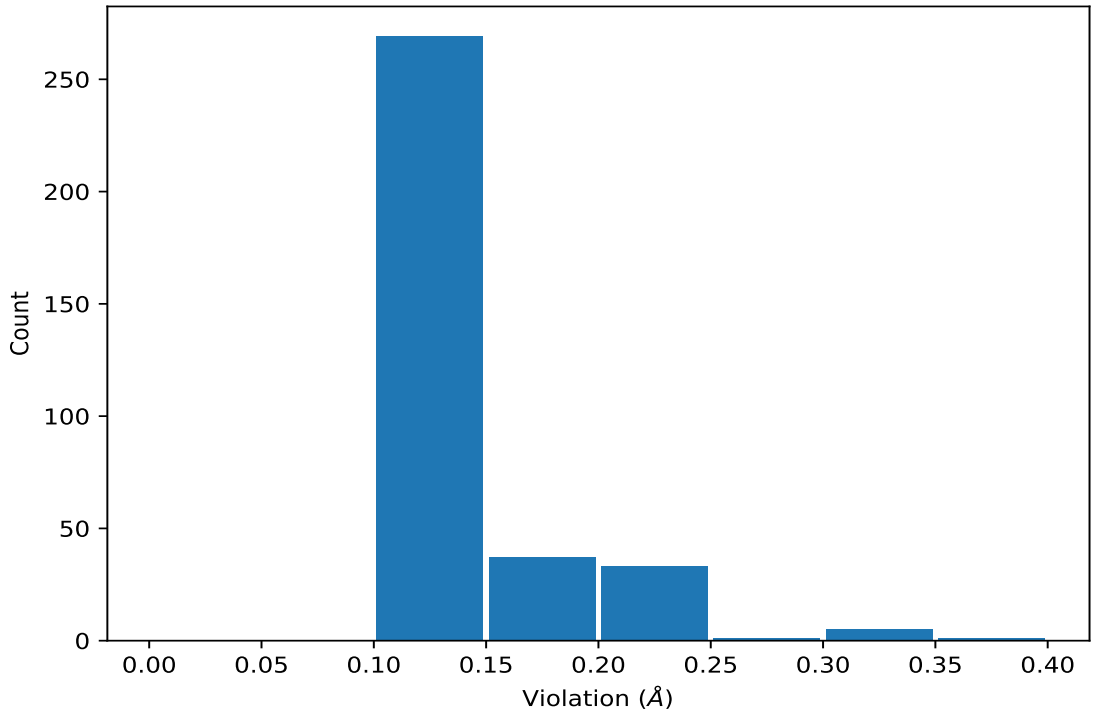
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	7	0.15	0.03	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	7	0.15	0.03	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	7	0.15	0.03	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	7	0.15	0.03	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	7	0.15	0.03	0.15
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	6	0.12	0.01	0.12
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	6	0.12	0.01	0.12
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	5	0.16	0.03	0.16
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	5	0.16	0.03	0.16
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	5	0.13	0.01	0.12
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	5	0.13	0.01	0.12
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	5	0.12	0.01	0.12
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	5	0.12	0.01	0.12
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	5	0.12	0.02	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	5	0.12	0.02	0.11
(2,13)	1:A:317:PHE:O	1:A:383:ARG:H	4	0.12	0.01	0.12
(1,491)	1:A:319:LEU:HD11	1:A:323:VAL:HB	3	0.14	0.01	0.14
(1,491)	1:A:319:LEU:HD12	1:A:323:VAL:HB	3	0.14	0.01	0.14
(1,491)	1:A:319:LEU:HD13	1:A:323:VAL:HB	3	0.14	0.01	0.14
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG11	3	0.12	0.01	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG12	3	0.12	0.01	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG13	3	0.12	0.01	0.11
(1,63)	1:A:316:LEU:HB2	1:A:384:SER:HB2	2	0.14	0.01	0.14
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD11	2	0.12	0.01	0.12
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD12	2	0.12	0.01	0.12
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD13	2	0.12	0.01	0.12
(1,275)	1:A:305:ARG:HA	1:A:305:ARG:HG2	2	0.12	0.0	0.12
(1,775)	1:A:352:PHE:HE1	1:A:353:ASN:HA	2	0.12	0.0	0.12
(1,775)	1:A:352:PHE:HE2	1:A:353:ASN:HA	2	0.12	0.0	0.12
(1,795)	1:A:352:PHE:HE1	1:A:353:ASN:HA	2	0.12	0.0	0.12
(1,795)	1:A:352:PHE:HE2	1:A:353:ASN:HA	2	0.12	0.0	0.12
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG12	2	0.11	0.0	0.11
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG13	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table 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)
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	12	0.37
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	2	0.35
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	7	0.34
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	4	0.33
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	14	0.33
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	9	0.31
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	17	0.3
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	11	0.24
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	19	0.24
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	17	0.23
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	17	0.23
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	1	0.23
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	13	0.23
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	9	0.23
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	2	0.22
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	18	0.22
(1,252)	1:A:373:ASN:HA	1:A:384:SER:HB2	20	0.22
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	4	0.21
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	5	0.21
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	7	0.21
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	12	0.21
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	20	0.21
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	4	0.21
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	17	0.21
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	3	0.2
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	8	0.2
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	10	0.2
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	14	0.2
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	2	0.2
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	2	0.2
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	2	0.2
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	2	0.2
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	2	0.2
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	2	0.2
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	7	0.2
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	12	0.2
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	14	0.2
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	20	0.2
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	20	0.2
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	6	0.19
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	16	0.19
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	17	0.19
(1,292)	1:A:312:THR:HG1	1:A:361:ASP:HA	4	0.19
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	12	0.19
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	12	0.19
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	16	0.18
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	16	0.18
(1,837)	1:A:331:PHE:H	1:A:334:GLU:HA	15	0.18
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	12	0.18
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	12	0.18
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	12	0.18
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	12	0.18
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	12	0.18
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	12	0.18
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	2	0.18
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	2	0.18
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	12	0.18
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	12	0.18
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	12	0.18
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	2	0.18
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	4	0.17
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	4	0.17
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	10	0.17
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	10	0.17
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	10	0.17
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	12	0.16
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	12	0.16
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	15	0.16
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	15	0.16
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	15	0.16
(1,491)	1:A:319:LEU:HD11	1:A:323:VAL:HB	10	0.16
(1,491)	1:A:319:LEU:HD12	1:A:323:VAL:HB	10	0.16
(1,491)	1:A:319:LEU:HD13	1:A:323:VAL:HB	10	0.16
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	8	0.16
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	8	0.16
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	14	0.15
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	20	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	1	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	1	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	3	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	3	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	8	0.15
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	8	0.15
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	14	0.15
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	14	0.15
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	5	0.15
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	5	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	1	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	1	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	1	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	1	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	1	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	1	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	3	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	3	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	3	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	3	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	3	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	13	0.15
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	13	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	13	0.15
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	13	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	13	0.15
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	13	0.15
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	14	0.15
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	14	0.15
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	14	0.15
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	17	0.15
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	17	0.15
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	17	0.15
(1,63)	1:A:316:LEU:HB2	1:A:384:SER:HB2	16	0.15
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	8	0.15
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	8	0.15
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	7	0.14
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	12	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	5	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	5	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	7	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	7	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	10	0.14
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	10	0.14
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	5	0.14
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	6	0.14
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	4	0.14
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	4	0.14
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	4	0.14
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	7	0.14
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	7	0.14
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	7	0.14
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	4	0.14
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	4	0.14
(1,491)	1:A:319:LEU:HD11	1:A:323:VAL:HB	5	0.14
(1,491)	1:A:319:LEU:HD12	1:A:323:VAL:HB	5	0.14
(1,491)	1:A:319:LEU:HD13	1:A:323:VAL:HB	5	0.14
(1,355)	1:A:344:ARG:HD2	1:A:358:ILE:HG12	5	0.14
(1,355)	1:A:344:ARG:HD2	1:A:358:ILE:HG13	5	0.14
(1,355)	1:A:344:ARG:HD3	1:A:358:ILE:HG12	5	0.14
(1,355)	1:A:344:ARG:HD3	1:A:358:ILE:HG13	5	0.14
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	15	0.14
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	8	0.14
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	8	0.14
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	8	0.14
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	12	0.14
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	12	0.14
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	12	0.14
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	17	0.14
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	17	0.14
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	17	0.14
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	18	0.14
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	18	0.14
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	18	0.14
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	20	0.14
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	20	0.14
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	20	0.14
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	10	0.14
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	10	0.14
(2,31)	1:A:308:LYS:O	1:A:312:THR:H	1	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	3	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	4	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	8	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	11	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	19	0.13
(2,13)	1:A:317:PHE:O	1:A:383:ARG:H	13	0.13
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	13	0.13
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	13	0.13
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	10	0.13
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	10	0.13
(1,734)	1:A:328:ILE:HG12	1:A:332:LEU:HD11	19	0.13
(1,734)	1:A:328:ILE:HG12	1:A:332:LEU:HD12	19	0.13
(1,734)	1:A:328:ILE:HG12	1:A:332:LEU:HD13	19	0.13
(1,734)	1:A:328:ILE:HG13	1:A:332:LEU:HD11	19	0.13
(1,734)	1:A:328:ILE:HG13	1:A:332:LEU:HD12	19	0.13
(1,734)	1:A:328:ILE:HG13	1:A:332:LEU:HD13	19	0.13
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	6	0.13
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	6	0.13
(1,703)	1:A:336:ILE:HG12	1:A:338:ILE:HG13	1	0.13
(1,703)	1:A:336:ILE:HG13	1:A:338:ILE:HG13	1	0.13
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG11	9	0.13
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG12	9	0.13
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG13	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	8	0.13
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	9	0.13
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	17	0.13
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	20	0.13
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	13	0.13
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	13	0.13
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	13	0.13
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	19	0.13
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	19	0.13
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	19	0.13
(1,63)	1:A:316:LEU:HB2	1:A:384:SER:HB2	13	0.13
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	9	0.13
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	9	0.13
(1,550)	1:A:344:ARG:HA	1:A:360:ARG:HG2	5	0.13
(1,491)	1:A:319:LEU:HD11	1:A:323:VAL:HB	7	0.13
(1,491)	1:A:319:LEU:HD12	1:A:323:VAL:HB	7	0.13
(1,491)	1:A:319:LEU:HD13	1:A:323:VAL:HB	7	0.13
(1,287)	1:A:350:SER:HB2	1:A:353:ASN:HA	8	0.13
(1,287)	1:A:350:SER:HB3	1:A:353:ASN:HA	8	0.13
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	16	0.13
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	16	0.13
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	14	0.13
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	14	0.13
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	11	0.13
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	11	0.13
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	11	0.13
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	13	0.13
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	13	0.13
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	13	0.13
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD11	9	0.13
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD12	9	0.13
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD13	9	0.13
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	3	0.13
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	3	0.13
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	11	0.13
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	11	0.13
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	13	0.13
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	13	0.13
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	2	0.12
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	13	0.12
(2,13)	1:A:317:PHE:O	1:A:383:ARG:H	10	0.12
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	2	0.12
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB2	15	0.12
(1,859)	1:A:318:PRO:HA	1:A:353:ASN:HB3	15	0.12
(1,795)	1:A:352:PHE:HE1	1:A:353:ASN:HA	13	0.12
(1,795)	1:A:352:PHE:HE2	1:A:353:ASN:HA	13	0.12
(1,775)	1:A:352:PHE:HE1	1:A:353:ASN:HA	13	0.12
(1,775)	1:A:352:PHE:HE2	1:A:353:ASN:HA	13	0.12
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	3	0.12
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	3	0.12
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	13	0.12
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	13	0.12
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	16	0.12
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	19	0.12
(1,654)	1:A:310:LEU:HD11	1:A:313:LEU:HG	9	0.12
(1,654)	1:A:310:LEU:HD12	1:A:313:LEU:HG	9	0.12
(1,654)	1:A:310:LEU:HD13	1:A:313:LEU:HG	9	0.12
(1,62)	1:A:384:SER:HB3	1:A:385:GLY:HA3	20	0.12
(1,578)	1:A:314:ILE:HG12	1:A:357:ILE:HD11	8	0.12
(1,578)	1:A:314:ILE:HG12	1:A:357:ILE:HD12	8	0.12
(1,578)	1:A:314:ILE:HG12	1:A:357:ILE:HD13	8	0.12
(1,578)	1:A:314:ILE:HG13	1:A:357:ILE:HD11	8	0.12
(1,578)	1:A:314:ILE:HG13	1:A:357:ILE:HD12	8	0.12
(1,578)	1:A:314:ILE:HG13	1:A:357:ILE:HD13	8	0.12
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	14	0.12
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	14	0.12
(1,275)	1:A:305:ARG:HA	1:A:305:ARG:HG2	7	0.12
(1,141)	1:A:312:THR:HG1	1:A:362:SER:HA	4	0.12
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	8	0.12
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	8	0.12
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	2	0.12
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	2	0.12
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	2	0.12
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	3	0.12
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	3	0.12
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	3	0.12
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	6	0.12
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	6	0.12
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	17	0.12
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	17	0.12
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	18	0.12
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	18	0.12
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	20	0.12
(2,43)	1:A:367:LYS:O	1:A:371:ILE:H	12	0.11
(2,23)	1:A:375:SER:H	1:A:382:ILE:O	10	0.11
(2,13)	1:A:317:PHE:O	1:A:383:ARG:H	16	0.11
(2,13)	1:A:317:PHE:O	1:A:383:ARG:H	18	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	2	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	2	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	12	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	12	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG12	20	0.11
(1,836)	1:A:359:PHE:H	1:A:338:ILE:HG13	20	0.11
(1,795)	1:A:352:PHE:HE1	1:A:353:ASN:HA	2	0.11
(1,795)	1:A:352:PHE:HE2	1:A:353:ASN:HA	2	0.11
(1,790)	1:A:394:TYR:HE1	1:A:397:GLN:HA	18	0.11
(1,790)	1:A:394:TYR:HE2	1:A:397:GLN:HA	18	0.11
(1,775)	1:A:352:PHE:HE1	1:A:353:ASN:HA	2	0.11
(1,775)	1:A:352:PHE:HE2	1:A:353:ASN:HA	2	0.11
(1,721)	1:A:357:ILE:HG12	1:A:358:ILE:HG12	5	0.11
(1,721)	1:A:357:ILE:HG12	1:A:358:ILE:HG13	5	0.11
(1,721)	1:A:357:ILE:HG13	1:A:358:ILE:HG12	5	0.11
(1,721)	1:A:357:ILE:HG13	1:A:358:ILE:HG13	5	0.11
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG12	10	0.11
(1,720)	1:A:312:THR:HG1	1:A:358:ILE:HG13	10	0.11
(1,702)	1:A:336:ILE:HG12	1:A:338:ILE:HB	17	0.11
(1,702)	1:A:336:ILE:HG13	1:A:338:ILE:HB	17	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG11	2	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG12	2	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG13	2	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG11	17	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG12	17	0.11
(1,677)	1:A:374:GLY:HA3	1:A:381:VAL:HG13	17	0.11
(1,669)	1:A:310:LEU:HB2	1:A:386:THR:HG1	19	0.11
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	12	0.11
(1,667)	1:A:314:ILE:HB	1:A:386:THR:HG1	15	0.11
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	19	0.11
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	19	0.11
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	19	0.11
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	19	0.11
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	19	0.11
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	19	0.11
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD1	20	0.11
(1,661)	1:A:298:VAL:HG11	1:A:352:PHE:HD2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD1	20	0.11
(1,661)	1:A:298:VAL:HG12	1:A:352:PHE:HD2	20	0.11
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD1	20	0.11
(1,661)	1:A:298:VAL:HG13	1:A:352:PHE:HD2	20	0.11
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	2	0.11
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	2	0.11
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	13	0.11
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	13	0.11
(1,577)	1:A:328:ILE:HG12	1:A:329:CYS:HB2	16	0.11
(1,577)	1:A:328:ILE:HG13	1:A:329:CYS:HB2	16	0.11
(1,275)	1:A:305:ARG:HA	1:A:305:ARG:HG2	8	0.11
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG12	5	0.11
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG13	5	0.11
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG12	13	0.11
(1,250)	1:A:345:LYS:HA	1:A:346:ILE:HG13	13	0.11
(1,237)	1:A:387:ILE:HG12	1:A:388:ASN:HA	2	0.11
(1,237)	1:A:387:ILE:HG13	1:A:388:ASN:HA	2	0.11
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	4	0.11
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	4	0.11
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG12	20	0.11
(1,132)	1:A:343:ILE:HA	1:A:357:ILE:HG13	20	0.11
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	1	0.11
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	1	0.11
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	1	0.11
(1,122)	1:A:313:LEU:HD11	1:A:358:ILE:HA	16	0.11
(1,122)	1:A:313:LEU:HD12	1:A:358:ILE:HA	16	0.11
(1,122)	1:A:313:LEU:HD13	1:A:358:ILE:HA	16	0.11
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD11	13	0.11
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD12	13	0.11
(1,106)	1:A:318:PRO:HA	1:A:319:LEU:HD13	13	0.11
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	7	0.11
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	7	0.11
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	9	0.11
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	9	0.11
(1,10)	1:A:392:ARG:HB2	1:A:393:TYR:HB3	16	0.11
(1,10)	1:A:392:ARG:HB3	1:A:393:TYR:HB3	16	0.11

10 Dihedral-angle violation analysis

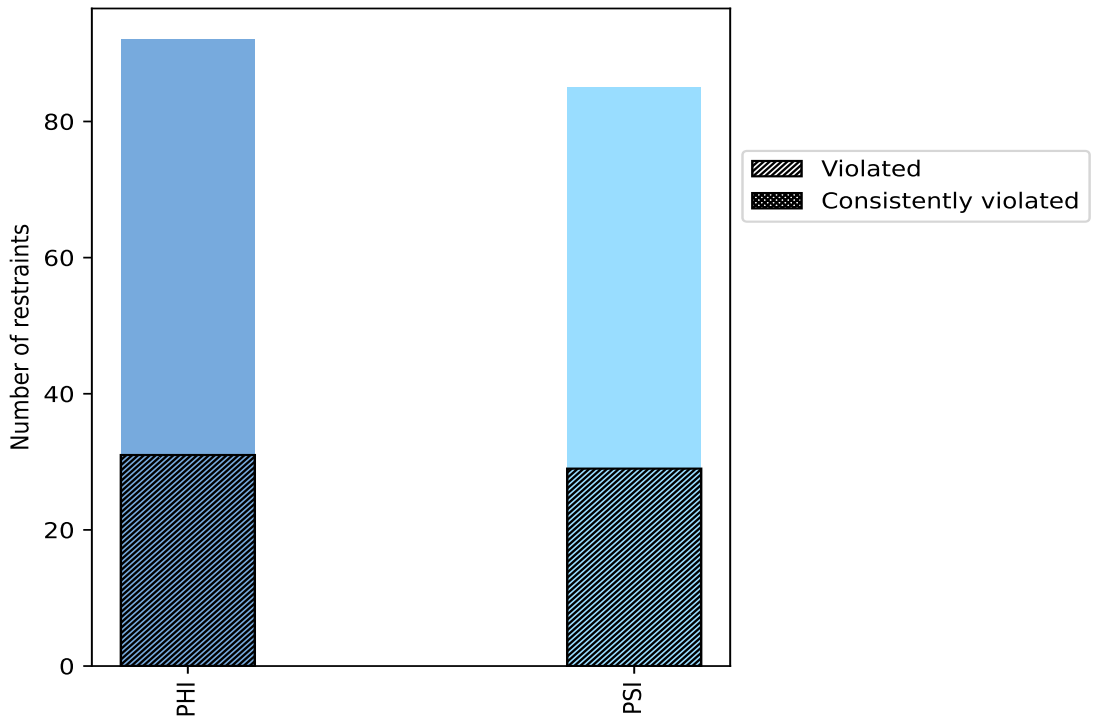
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	92	52.0	31	33.7	17.5	0	0.0	0.0
PSI	85	48.0	29	34.1	16.4	0	0.0	0.0
Total	177	100.0	60	33.9	33.9	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



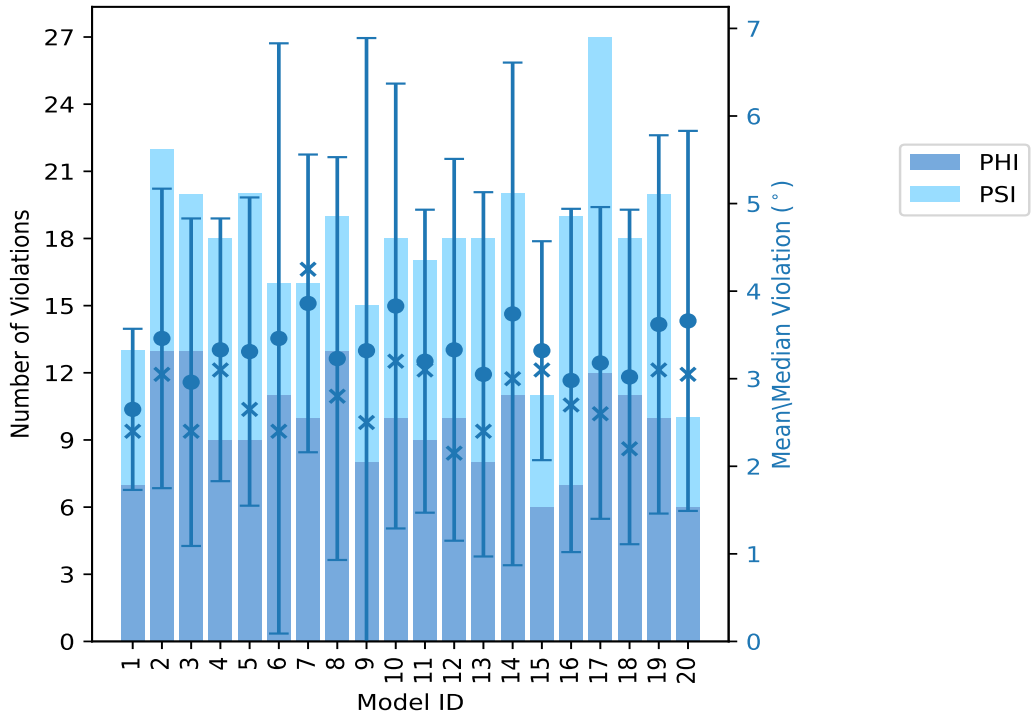
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	7	6	13	2.65	4.9	0.92	2.4
2	13	9	22	3.46	7.5	1.71	3.05
3	13	7	20	2.96	9.1	1.87	2.4
4	9	9	18	3.33	7.2	1.5	3.1
5	9	11	20	3.31	6.8	1.76	2.65
6	11	5	16	3.46	14.3	3.37	2.4
7	10	6	16	3.86	6.8	1.7	4.25
8	13	6	19	3.23	11.0	2.3	2.8
9	8	7	15	3.32	16.2	3.57	2.5
10	10	8	18	3.83	12.7	2.54	3.2
11	9	8	17	3.2	8.1	1.73	3.1
12	10	8	18	3.33	8.6	2.18	2.15
13	8	10	18	3.05	9.0	2.08	2.4
14	11	9	20	3.74	11.2	2.87	3.0
15	6	5	11	3.32	5.9	1.25	3.1
16	7	12	19	2.98	9.4	1.96	2.7
17	12	15	27	3.18	9.2	1.78	2.6
18	11	7	18	3.02	9.1	1.91	2.2
19	10	10	20	3.62	9.2	2.16	3.1
20	6	4	10	3.66	7.3	2.17	3.05

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
9	5	14	1	5.0
7	5	12	2	10.0
1	3	4	3	15.0
0	1	1	4	20.0
0	1	1	5	25.0
1	4	5	6	30.0
0	1	1	7	35.0
0	1	1	8	40.0
2	2	4	9	45.0
0	2	2	10	50.0
1	1	2	11	55.0

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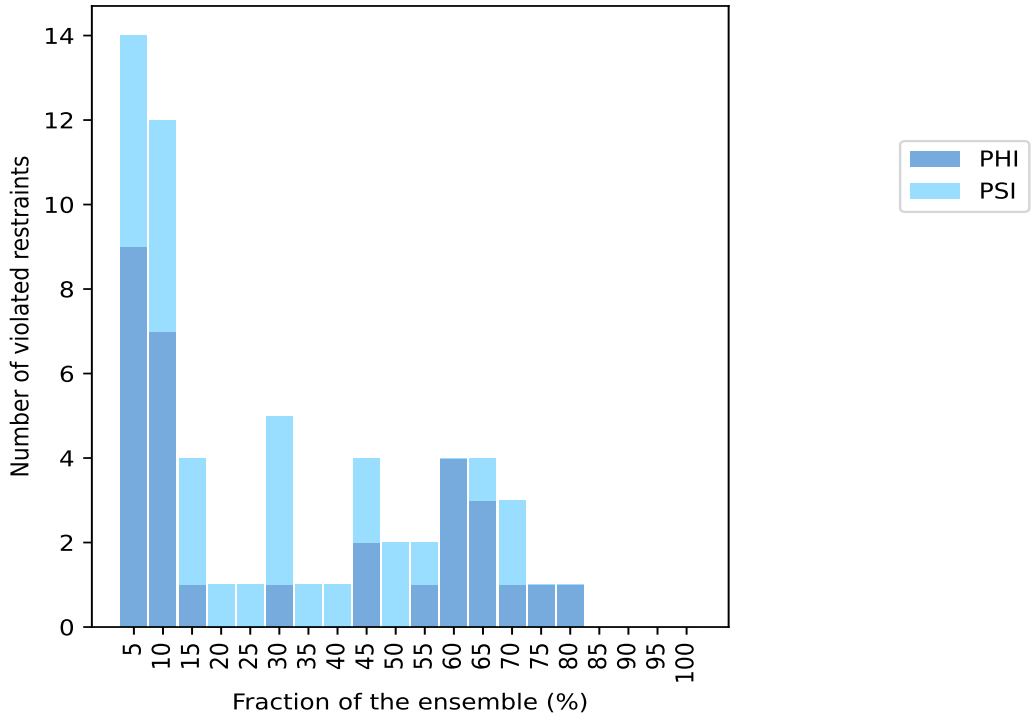
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
4	0	4	12	60.0
3	1	4	13	65.0
1	2	3	14	70.0
1	0	1	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

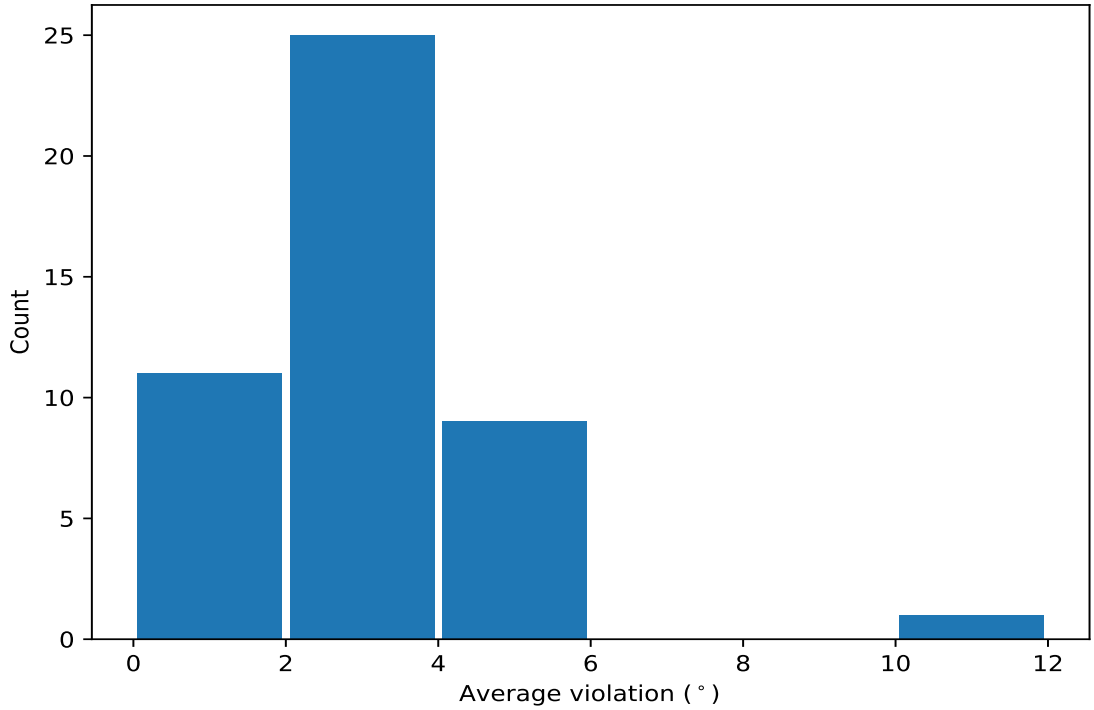


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	16	4.54	3.79	3.35
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	15	4.63	1.68	4.3
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	14	3.76	2.45	3.1
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	14	3.05	1.38	2.6
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	14	2.66	1.12	2.3
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	13	4.75	2.48	5.4
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	13	4.54	2.39	3.7
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	13	3.72	1.18	3.5
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	13	2.48	0.82	2.2
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	12	3.42	1.04	3.45
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	12	3.37	1.39	3.3
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	12	3.15	1.09	3.25
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	12	2.34	1.05	2.3
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	11	4.44	1.85	4.4
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	11	3.25	1.22	2.7
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	10	5.55	2.76	5.6
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	10	2.23	0.96	1.95
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	9	4.48	2.6	4.1
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	9	2.39	1.25	1.9
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	9	2.24	0.55	2.4

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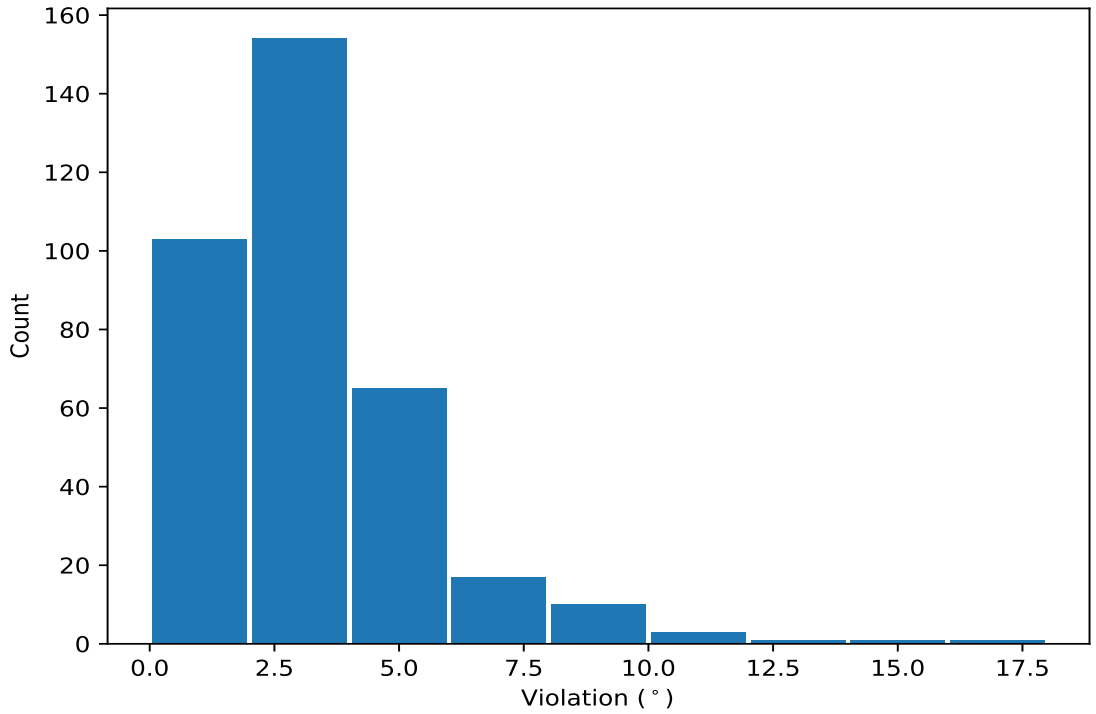
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	9	2.12	0.72	1.8
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	8	2.43	1.22	1.95
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	7	2.3	0.69	2.1
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	6	10.48	2.22	9.3
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	6	4.32	1.53	4.65
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	6	3.0	1.22	3.3
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	6	2.65	0.82	2.4
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	6	1.83	0.7	1.6
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	5	2.18	0.31	2.3
(1,50)	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1:A:326:SER:N	4	1.5	0.46	1.25
(1,76)	1:A:338:ILE:N	1:A:338:ILE:CA	1:A:338:ILE:C	1:A:339:ASN:N	3	2.77	0.48	3.0
(1,107)	1:A:358:ILE:N	1:A:358:ILE:CA	1:A:358:ILE:C	1:A:359:PHE:N	3	2.77	0.56	3.0
(1,148)	1:A:383:ARG:C	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	3	1.97	0.24	1.8
(1,18)	1:A:302:LEU:N	1:A:302:LEU:CA	1:A:302:LEU:C	1:A:303:ALA:N	3	1.17	0.05	1.2
(1,97)	1:A:348:LEU:C	1:A:349:VAL:N	1:A:349:VAL:CA	1:A:349:VAL:C	2	4.2	0.8	4.2
(1,2)	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	1:A:295:ARG:N	2	2.95	1.75	2.95
(1,95)	1:A:347:LEU:C	1:A:348:LEU:N	1:A:348:LEU:CA	1:A:348:LEU:C	2	2.8	0.4	2.8
(1,66)	1:A:333:GLN:N	1:A:333:GLN:CA	1:A:333:GLN:C	1:A:334:GLU:N	2	2.15	0.45	2.15
(1,41)	1:A:319:LEU:C	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	2	2.0	0.7	2.0
(1,143)	1:A:380:LYS:C	1:A:381:VAL:N	1:A:381:VAL:CA	1:A:381:VAL:C	2	1.9	0.3	1.9
(1,80)	1:A:340:GLU:N	1:A:340:GLU:CA	1:A:340:GLU:C	1:A:341:LYS:N	2	1.65	0.15	1.65
(1,152)	1:A:385:GLY:C	1:A:386:THR:N	1:A:386:THR:CA	1:A:386:THR:C	2	1.55	0.25	1.55
(1,155)	1:A:387:ILE:C	1:A:388:ASN:N	1:A:388:ASN:CA	1:A:388:ASN:C	2	1.55	0.15	1.55
(1,33)	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	1:A:314:ILE:N	2	1.5	0.3	1.5
(1,1)	1:A:293:LEU:C	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	2	1.45	0.25	1.45
(1,14)	1:A:300:ARG:N	1:A:300:ARG:CA	1:A:300:ARG:C	1:A:301:LEU:N	2	1.4	0.3	1.4

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	9	16.2
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	6	14.3
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	10	12.7
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	14	11.2
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	8	11.0
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	14	10.7
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	16	9.4
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	6	9.2
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	17	9.2
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	19	9.2
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	18	9.1
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	3	9.1
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	13	9.0
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	12	8.6
(1,108)	1:A:360:ARG:N	1:A:360:ARG:CA	1:A:360:ARG:C	1:A:361:ASP:N	11	8.1
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	13	8.0
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	19	7.8
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	10	7.6
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	12	7.6
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	17	7.6
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	2	7.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	20	7.3
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	4	7.2
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	14	6.8
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	5	6.8
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	7	6.8
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	14	6.3
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	5	6.3
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	7	6.2
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	20	6.2
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	2	6.1
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	3	6.1
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	19	6.1
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	15	5.9
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	20	5.9
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	12	5.8
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	18	5.8
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	2	5.7
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	12	5.6
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	5	5.6
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	8	5.6
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	2	5.5
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	8	5.5
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	7	5.4
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	18	5.3
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	11	5.3
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	7	5.2
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	2	5.1
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	4	5.1
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	7	5.1
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	19	5.1
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	4	5.1
(1,105)	1:A:357:ILE:N	1:A:357:ILE:CA	1:A:357:ILE:C	1:A:358:ILE:N	5	5.1
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	16	5.1
(1,97)	1:A:348:LEU:C	1:A:349:VAL:N	1:A:349:VAL:CA	1:A:349:VAL:C	8	5.0
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	3	5.0
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	2	5.0
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	20	5.0
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	15	4.9
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	1	4.9
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	17	4.9
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	10	4.9
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	5	4.9
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	4	4.9
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	12	4.8
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	5	4.7
(1,2)	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	1:A:295:ARG:N	19	4.7
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	17	4.7
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	19	4.7
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	5	4.6
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	11	4.6
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	9	4.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	2	4.6
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	7	4.6
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	13	4.5
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	10	4.5
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	11	4.4
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	17	4.4
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	16	4.4
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	19	4.4
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	7	4.4
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	14	4.4
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	7	4.3
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	11	4.3
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	3	4.3
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	14	4.2
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	15	4.2
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	7	4.2
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	19	4.2
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	16	4.2
(1,104)	1:A:356:ILE:C	1:A:357:ILE:N	1:A:357:ILE:CA	1:A:357:ILE:C	5	4.2
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	17	4.1
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	18	4.1
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	8	4.1
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	4	4.1
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	2	4.1
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	6	4.1
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	16	4.0
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	10	3.9
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	4	3.9
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	4	3.9
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	14	3.9
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	10	3.7
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	19	3.7
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	12	3.7
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	16	3.7
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	6	3.7
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	7	3.7
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	7	3.7
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	20	3.7
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	11	3.6
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	10	3.6
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	16	3.5
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	9	3.5
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	9	3.5
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	17	3.5
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	15	3.5
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	14	3.5
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	1	3.5
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	5	3.5
(1,97)	1:A:348:LEU:C	1:A:349:VAL:N	1:A:349:VAL:CA	1:A:349:VAL:C	17	3.4
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	17	3.4
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	14	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	1	3.4
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	10	3.4
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	15	3.4
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	11	3.4
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	17	3.4
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	16	3.3
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	4	3.3
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	19	3.3
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	2	3.3
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	9	3.3
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	2	3.3
(1,107)	1:A:358:ILE:N	1:A:358:ILE:CA	1:A:358:ILE:C	1:A:359:PHE:N	14	3.3
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	12	3.3
(1,95)	1:A:347:LEU:C	1:A:348:LEU:N	1:A:348:LEU:CA	1:A:348:LEU:C	8	3.2
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	10	3.2
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	3	3.2
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	18	3.2
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	8	3.2
(1,76)	1:A:338:ILE:N	1:A:338:ILE:CA	1:A:338:ILE:C	1:A:339:ASN:N	16	3.2
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	2	3.2
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	10	3.2
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	6	3.2
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	13	3.2
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	17	3.2
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	15	3.1
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	1	3.1
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	4	3.1
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	3	3.1
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	4	3.1
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	8	3.1
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	18	3.1
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	11	3.1
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	11	3.1
(1,76)	1:A:338:ILE:N	1:A:338:ILE:CA	1:A:338:ILE:C	1:A:339:ASN:N	15	3.0
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1	3.0
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	10	3.0
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	13	3.0
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	8	3.0
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	17	3.0
(1,107)	1:A:358:ILE:N	1:A:358:ILE:CA	1:A:358:ILE:C	1:A:359:PHE:N	4	3.0
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	3	2.9
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	13	2.9
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	19	2.9
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	2	2.9
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	12	2.9
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	13	2.9
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	3	2.8
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	19	2.8
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	19	2.8
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	5	2.8
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	8	2.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	1	2.8
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	15	2.8
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	10	2.8
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	11	2.7
(1,41)	1:A:319:LEU:C	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	3	2.7
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	14	2.7
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	2	2.7
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	16	2.7
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	6	2.7
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	17	2.7
(1,75)	1:A:337:HIS:C	1:A:338:ILE:N	1:A:338:ILE:CA	1:A:338:ILE:C	2	2.6
(1,66)	1:A:333:GLN:N	1:A:333:GLN:CA	1:A:333:GLN:C	1:A:334:GLU:N	17	2.6
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	6	2.6
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	13	2.6
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	9	2.6
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	9	2.6
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	17	2.6
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	8	2.6
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	11	2.5
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	13	2.5
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	6	2.5
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	5	2.5
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	10	2.5
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	3	2.5
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	9	2.5
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	17	2.4
(1,95)	1:A:347:LEU:C	1:A:348:LEU:N	1:A:348:LEU:CA	1:A:348:LEU:C	17	2.4
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	2	2.4
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	18	2.4
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	17	2.4
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	20	2.4
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	4	2.4
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	10	2.4
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	1	2.4
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	2	2.4
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	3	2.3
(1,50)	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1:A:326:SER:N	1	2.3
(1,45)	1:A:321:ASP:C	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	18	2.3
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	6	2.3
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	12	2.3
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	4	2.3
(1,148)	1:A:383:ARG:C	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	13	2.3
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	8	2.3
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	17	2.3
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	15	2.3
(1,84)	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	1:A:343:ILE:N	13	2.2
(1,49)	1:A:324:SER:C	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1	2.2
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	6	2.2
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	2	2.2
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	20	2.2
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	17	2.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	18	2.2
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	18	2.2
(1,143)	1:A:380:LYS:C	1:A:381:VAL:N	1:A:381:VAL:CA	1:A:381:VAL:C	18	2.2
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	8	2.2
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	5	2.2
(1,135)	1:A:376:GLN:C	1:A:377:PHE:N	1:A:377:PHE:CA	1:A:377:PHE:C	14	2.2
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	15	2.2
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	13	2.2
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	4	2.2
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	1	2.1
(1,76)	1:A:338:ILE:N	1:A:338:ILE:CA	1:A:338:ILE:C	1:A:339:ASN:N	17	2.1
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	18	2.1
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	13	2.1
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	3	2.1
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	19	2.1
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	9	2.1
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	5	2.0
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	12	2.0
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	14	2.0
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	3	2.0
(1,153)	1:A:386:THR:C	1:A:387:ILE:N	1:A:387:ILE:CA	1:A:387:ILE:C	12	2.0
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	7	2.0
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	3	2.0
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	16	2.0
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	10	2.0
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	10	2.0
(1,107)	1:A:358:ILE:N	1:A:358:ILE:CA	1:A:358:ILE:C	1:A:359:PHE:N	17	2.0
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	9	1.9
(1,78)	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	1:A:340:GLU:N	18	1.9
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	2	1.9
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	18	1.9
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	11	1.9
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	18	1.9
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	11	1.9
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	18	1.9
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	12	1.9
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	5	1.9
(1,130)	1:A:372:LEU:N	1:A:372:LEU:CA	1:A:372:LEU:C	1:A:373:ASN:N	5	1.9
(1,99)	1:A:349:VAL:C	1:A:350:SER:N	1:A:350:SER:CA	1:A:350:SER:C	4	1.8
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	12	1.8
(1,80)	1:A:340:GLU:N	1:A:340:GLU:CA	1:A:340:GLU:C	1:A:341:LYS:N	9	1.8
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	10	1.8
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	2	1.8
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	3	1.8
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	1	1.8
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	14	1.8
(1,33)	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	1:A:314:ILE:N	11	1.8
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	17	1.8
(1,152)	1:A:385:GLY:C	1:A:386:THR:N	1:A:386:THR:CA	1:A:386:THR:C	6	1.8
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	12	1.8
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	14	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:A:383:ARG:C	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	3	1.8
(1,148)	1:A:383:ARG:C	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	19	1.8
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	13	1.8
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	7	1.8
(1,102)	1:A:355:ALA:C	1:A:356:ILE:N	1:A:356:ILE:CA	1:A:356:ILE:C	4	1.8
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	10	1.7
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	12	1.7
(1,66)	1:A:333:GLN:N	1:A:333:GLN:CA	1:A:333:GLN:C	1:A:334:GLU:N	16	1.7
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	8	1.7
(1,35)	1:A:314:ILE:N	1:A:314:ILE:CA	1:A:314:ILE:C	1:A:315:CYS:N	5	1.7
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	3	1.7
(1,32)	1:A:312:THR:C	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	16	1.7
(1,155)	1:A:387:ILE:C	1:A:388:ASN:N	1:A:388:ASN:CA	1:A:388:ASN:C	13	1.7
(1,14)	1:A:300:ARG:N	1:A:300:ARG:CA	1:A:300:ARG:C	1:A:301:LEU:N	5	1.7
(1,100)	1:A:352:PHE:N	1:A:352:PHE:CA	1:A:352:PHE:C	1:A:353:ASN:N	1	1.7
(1,1)	1:A:293:LEU:C	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	13	1.7
(1,81)	1:A:340:GLU:C	1:A:341:LYS:N	1:A:341:LYS:CA	1:A:341:LYS:C	6	1.6
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	6	1.6
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	7	1.6
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	16	1.6
(1,31)	1:A:310:LEU:C	1:A:311:GLU:N	1:A:311:GLU:CA	1:A:311:GLU:C	17	1.6
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	19	1.6
(1,143)	1:A:380:LYS:C	1:A:381:VAL:N	1:A:381:VAL:CA	1:A:381:VAL:C	12	1.6
(1,138)	1:A:378:GLN:N	1:A:378:GLN:CA	1:A:378:GLN:C	1:A:379:GLY:N	3	1.6
(1,110)	1:A:362:SER:N	1:A:362:SER:CA	1:A:362:SER:C	1:A:363:LYS:N	14	1.6
(1,80)	1:A:340:GLU:N	1:A:340:GLU:CA	1:A:340:GLU:C	1:A:341:LYS:N	17	1.5
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	9	1.5
(1,141)	1:A:379:GLY:C	1:A:380:LYS:N	1:A:380:LYS:CA	1:A:380:LYS:C	8	1.5
(1,140)	1:A:379:GLY:N	1:A:379:GLY:CA	1:A:379:GLY:C	1:A:380:LYS:N	18	1.5
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	7	1.4
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	19	1.4
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	4	1.4
(1,77)	1:A:338:ILE:C	1:A:339:ASN:N	1:A:339:ASN:CA	1:A:339:ASN:C	9	1.4
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	14	1.4
(1,46)	1:A:322:LYS:N	1:A:322:LYS:CA	1:A:322:LYS:C	1:A:323:VAL:N	4	1.4
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	2	1.4
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	19	1.4
(1,37)	1:A:315:CYS:C	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	5	1.4
(1,155)	1:A:387:ILE:C	1:A:388:ASN:N	1:A:388:ASN:CA	1:A:388:ASN:C	6	1.4
(1,147)	1:A:383:ARG:N	1:A:383:ARG:CA	1:A:383:ARG:C	1:A:384:SER:N	20	1.4
(1,83)	1:A:341:LYS:C	1:A:342:ASP:N	1:A:342:ASP:CA	1:A:342:ASP:C	16	1.3
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	14	1.3
(1,50)	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1:A:326:SER:N	19	1.3
(1,41)	1:A:319:LEU:C	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	20	1.3
(1,28)	1:A:308:LYS:C	1:A:309:GLU:N	1:A:309:GLU:CA	1:A:309:GLU:C	17	1.3
(1,152)	1:A:385:GLY:C	1:A:386:THR:N	1:A:386:THR:CA	1:A:386:THR:C	12	1.3
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	7	1.3
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	11	1.3
(1,89)	1:A:344:ARG:C	1:A:345:LYS:N	1:A:345:LYS:CA	1:A:345:LYS:C	2	1.2
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	11	1.2
(1,69)	1:A:334:GLU:C	1:A:335:GLU:N	1:A:335:GLU:CA	1:A:335:GLU:C	8	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1:A:326:SER:N	2	1.2
(1,50)	1:A:325:PRO:N	1:A:325:PRO:CA	1:A:325:PRO:C	1:A:326:SER:N	5	1.2
(1,43)	1:A:320:SER:C	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	12	1.2
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	16	1.2
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	20	1.2
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	1	1.2
(1,38)	1:A:316:LEU:N	1:A:316:LEU:CA	1:A:316:LEU:C	1:A:317:PHE:N	16	1.2
(1,33)	1:A:313:LEU:N	1:A:313:LEU:CA	1:A:313:LEU:C	1:A:314:ILE:N	18	1.2
(1,25)	1:A:307:SER:N	1:A:307:SER:CA	1:A:307:SER:C	1:A:308:LYS:N	5	1.2
(1,2)	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	1:A:295:ARG:N	13	1.2
(1,18)	1:A:302:LEU:N	1:A:302:LEU:CA	1:A:302:LEU:C	1:A:303:ALA:N	11	1.2
(1,18)	1:A:302:LEU:N	1:A:302:LEU:CA	1:A:302:LEU:C	1:A:303:ALA:N	16	1.2
(1,149)	1:A:384:SER:N	1:A:384:SER:CA	1:A:384:SER:C	1:A:385:GLY:N	19	1.2
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	8	1.2
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	15	1.2
(1,132)	1:A:374:GLY:C	1:A:375:SER:N	1:A:375:SER:CA	1:A:375:SER:C	16	1.2
(1,1)	1:A:293:LEU:C	1:A:294:GLU:N	1:A:294:GLU:CA	1:A:294:GLU:C	9	1.2
(1,72)	1:A:336:ILE:N	1:A:336:ILE:CA	1:A:336:ILE:C	1:A:337:HIS:N	14	1.1
(1,62)	1:A:331:PHE:N	1:A:331:PHE:CA	1:A:331:PHE:C	1:A:332:LEU:N	6	1.1
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	8	1.1
(1,60)	1:A:330:GLN:N	1:A:330:GLN:CA	1:A:330:GLN:C	1:A:331:PHE:N	17	1.1
(1,44)	1:A:321:ASP:N	1:A:321:ASP:CA	1:A:321:ASP:C	1:A:322:LYS:N	13	1.1
(1,42)	1:A:320:SER:N	1:A:320:SER:CA	1:A:320:SER:C	1:A:321:ASP:N	8	1.1
(1,18)	1:A:302:LEU:N	1:A:302:LEU:CA	1:A:302:LEU:C	1:A:303:ALA:N	14	1.1
(1,145)	1:A:381:VAL:C	1:A:382:ILE:N	1:A:382:ILE:CA	1:A:382:ILE:C	3	1.1
(1,14)	1:A:300:ARG:N	1:A:300:ARG:CA	1:A:300:ARG:C	1:A:301:LEU:N	9	1.1
(1,131)	1:A:372:LEU:C	1:A:373:ASN:N	1:A:373:ASN:CA	1:A:373:ASN:C	3	1.1
(1,117)	1:A:365:ALA:C	1:A:366:ALA:N	1:A:366:ALA:CA	1:A:366:ALA:C	6	1.1