



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:13 AM UTC

PDB ID : 7KNV / pdb_00007knv
BMRB ID : 30812
Title : Solution NMR structure of CDHR3 extracellular domain EC1
Authors : Lee, W.; Tonelli, M.; Frederick, R.O.; Watters, K.E.; Markley, J.L.; Palmenberg, A.C.
Deposited on : 2020-11-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

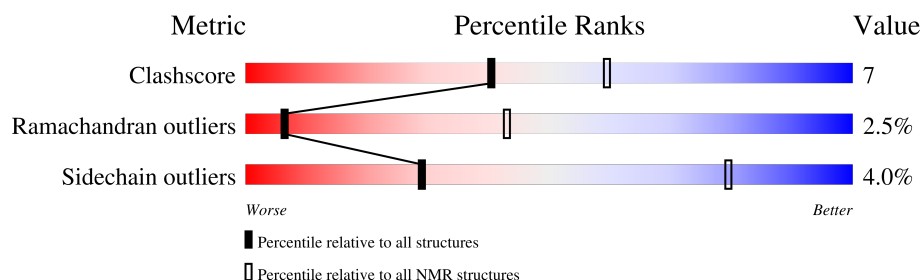
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	126	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:20-A:126 (107)	0.89	13

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1914 atoms, of which 946 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cadherin-related family member 3.

Mol	Chain	Residues	Atoms						Trace
1	A	126	Total	C	H	N	O	S	0
			1911	615	946	152	196	2	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q6ZTQ4
A	10	ALA	-	expression tag	UNP Q6ZTQ4
A	11	SER	-	expression tag	UNP Q6ZTQ4
A	12	ASP	-	expression tag	UNP Q6ZTQ4
A	13	TYR	-	expression tag	UNP Q6ZTQ4
A	14	LYS	-	expression tag	UNP Q6ZTQ4
A	15	ASP	-	expression tag	UNP Q6ZTQ4
A	16	ASP	-	expression tag	UNP Q6ZTQ4
A	17	ASP	-	expression tag	UNP Q6ZTQ4
A	18	ASP	-	expression tag	UNP Q6ZTQ4
A	19	LYS	-	expression tag	UNP Q6ZTQ4
A	20	LEU	-	expression tag	UNP Q6ZTQ4
A	131	GLY	-	expression tag	UNP Q6ZTQ4
A	132	GLY	-	expression tag	UNP Q6ZTQ4
A	133	THR	-	expression tag	UNP Q6ZTQ4
A	134	LYS	-	expression tag	UNP Q6ZTQ4

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

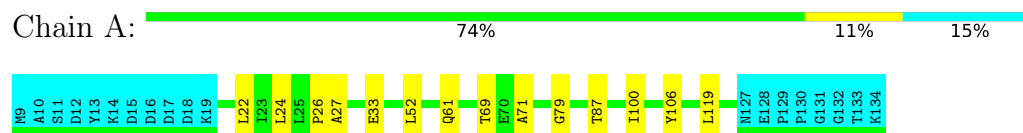
Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Cadherin-related family member 3

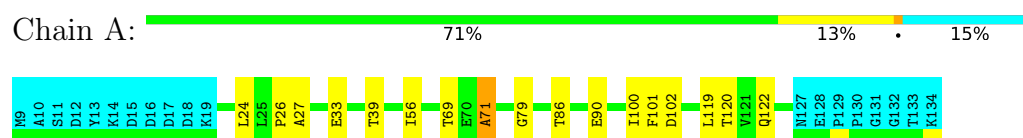


4.2 Scores per residue for each member of the ensemble

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

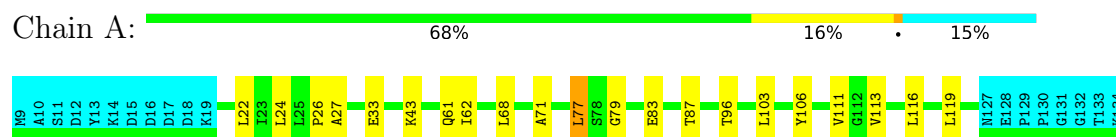
4.2.1 Score per residue for model 1

- Molecule 1: Cadherin-related family member 3



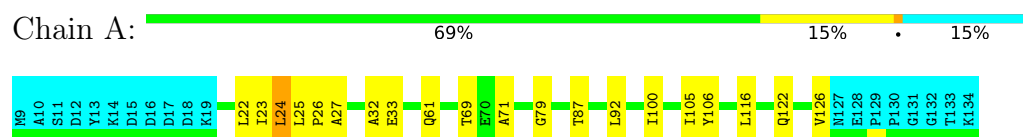
4.2.2 Score per residue for model 2

- Molecule 1: Cadherin-related family member 3



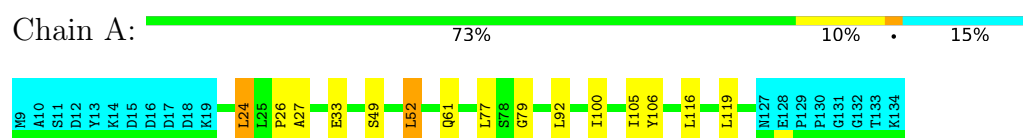
4.2.3 Score per residue for model 3

- Molecule 1: Cadherin-related family member 3



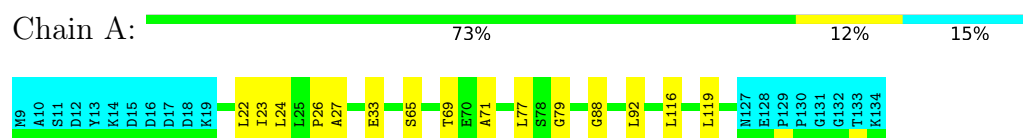
4.2.4 Score per residue for model 4

- Molecule 1: Cadherin-related family member 3



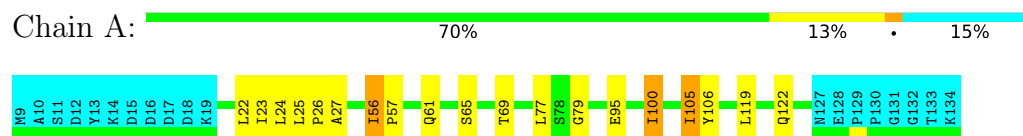
4.2.5 Score per residue for model 5

- Molecule 1: Cadherin-related family member 3



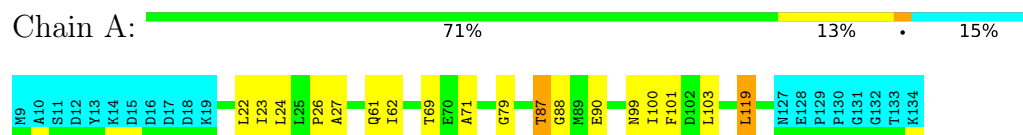
4.2.6 Score per residue for model 6

- Molecule 1: Cadherin-related family member 3



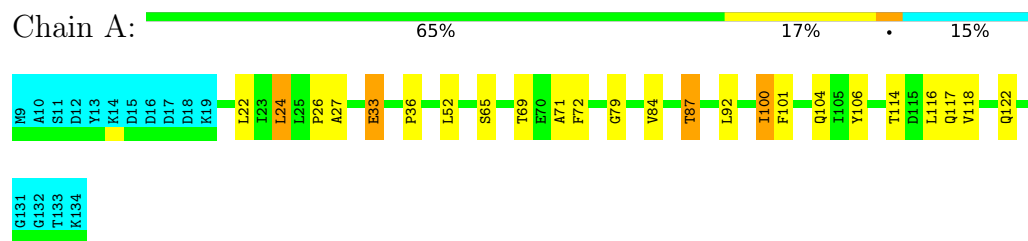
4.2.7 Score per residue for model 7

- Molecule 1: Cadherin-related family member 3



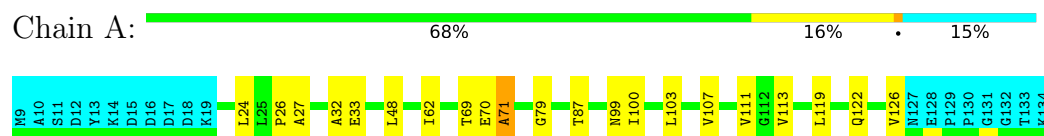
4.2.8 Score per residue for model 8

- Molecule 1: Cadherin-related family member 3



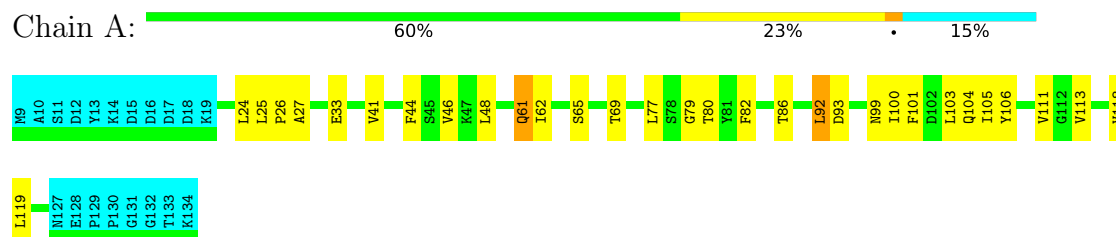
4.2.9 Score per residue for model 9

- Molecule 1: Cadherin-related family member 3



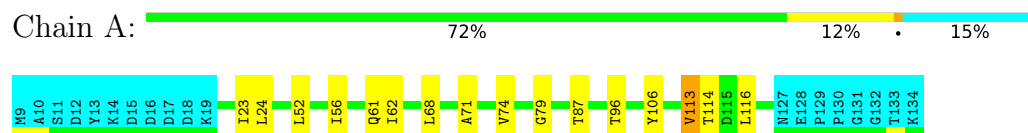
4.2.10 Score per residue for model 10

- Molecule 1: Cadherin-related family member 3



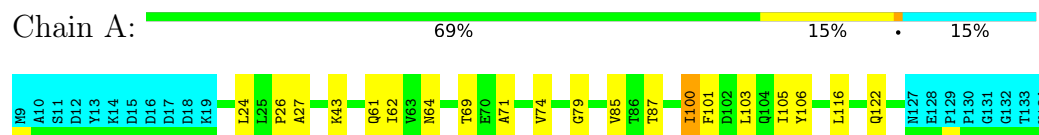
4.2.11 Score per residue for model 11

- Molecule 1: Cadherin-related family member 3



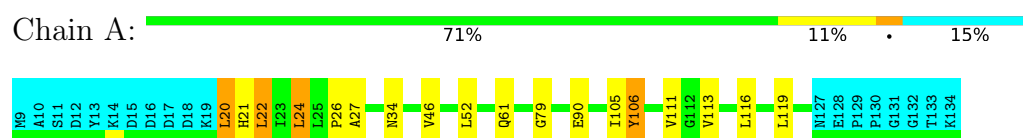
4.2.12 Score per residue for model 12

- Molecule 1: Cadherin-related family member 3



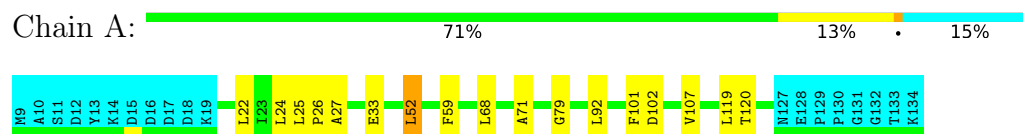
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Cadherin-related family member 3



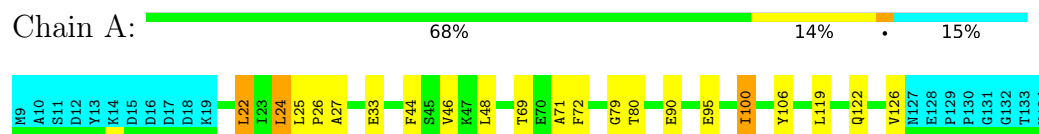
4.2.14 Score per residue for model 14

- Molecule 1: Cadherin-related family member 3



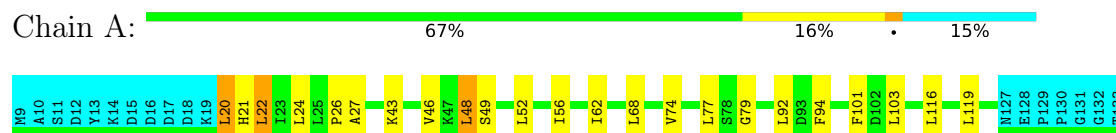
4.2.15 Score per residue for model 15

- Molecule 1: Cadherin-related family member 3



4.2.16 Score per residue for model 16

- Molecule 1: Cadherin-related family member 3



K134

4.2.17 Score per residue for model 17

- Molecule 1: Cadherin-related family member 3

Chain A: 



4.2.18 Score per residue for model 18

- Molecule 1: Cadherin-related family member 3

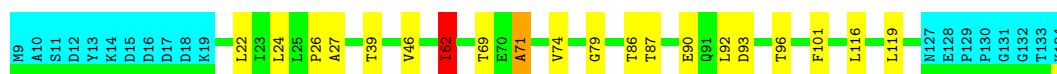
Chain A: 

T133
K134

4.2.19 Score per residue for model 19

- Molecule 1: Cadherin-related family member 3

Chain A: 



4.2.20 Score per residue for model 20

- Molecule 1: Cadherin-related family member 3

Chain A: 



K134

5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
PONDEROSA-C/S	structure calculation	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1403
Number of shifts mapped to atoms	1403
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.99±0.02	0±0/840 (0.0± 0.0%)	0.93±0.01	0±0/1155 (0.0± 0.0%)
All	All	0.99	3/16800 (0.0%)	0.93	0/23100 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	62	ILE	CA-CB	6.17	1.60	1.53	19	1
1	A	113	VAL	CA-CB	5.42	1.59	1.54	11	1
1	A	105	ILE	CA-CB	5.12	1.60	1.54	6	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	820	818	818	11±3
All	All	16460	16360	16360	229

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:THR:HG23	1:A:101:PHE:CE1	0.71	2.21	12	2
1:A:102:ASP:OD1	1:A:120:THR:HG22	0.70	1.87	17	2
1:A:71:ALA:HB1	1:A:87:THR:C	0.68	2.13	11	4
1:A:69:THR:HG22	1:A:72:PHE:CE2	0.66	2.25	15	1
1:A:71:ALA:HB2	1:A:90:GLU:O	0.66	1.91	18	6
1:A:26:PRO:HB3	1:A:27:ALA:HB2	0.65	1.67	19	3
1:A:65:SER:HB3	1:A:69:THR:HG21	0.64	1.69	10	4
1:A:71:ALA:HB1	1:A:87:THR:H	0.64	1.52	19	3
1:A:31:VAL:HG23	1:A:41:VAL:HG23	0.63	1.68	18	1
1:A:71:ALA:HB1	1:A:87:THR:O	0.63	1.94	11	2
1:A:93:ASP:O	1:A:96:THR:HG22	0.62	1.95	19	1
1:A:39:THR:O	1:A:86:THR:HG22	0.61	1.94	1	3
1:A:26:PRO:CB	1:A:27:ALA:HB2	0.61	2.25	2	18
1:A:31:VAL:CG1	1:A:41:VAL:HG22	0.61	2.24	20	1
1:A:62:ILE:HD11	1:A:74:VAL:HG23	0.59	1.75	12	2
1:A:68:LEU:HD21	1:A:92:LEU:HD12	0.58	1.73	16	1
1:A:22:LEU:HD23	1:A:46:VAL:HG22	0.56	1.76	13	1
1:A:48:LEU:HD23	1:A:80:THR:HG21	0.56	1.77	18	1
1:A:61:GLN:O	1:A:105:ILE:HG23	0.56	2.01	10	5
1:A:48:LEU:HD23	1:A:80:THR:HG22	0.56	1.76	10	1
1:A:119:LEU:O	1:A:119:LEU:HD13	0.56	2.01	17	1
1:A:102:ASP:OD2	1:A:120:THR:HG22	0.55	2.01	20	2
1:A:27:ALA:HB3	1:A:119:LEU:HA	0.54	1.78	6	4
1:A:34:ASN:ND2	1:A:71:ALA:HB3	0.54	2.17	17	1
1:A:69:THR:HG22	1:A:72:PHE:CD2	0.54	2.38	15	1
1:A:71:ALA:HB3	1:A:92:LEU:HG	0.54	1.80	19	2
1:A:49:SER:O	1:A:52:LEU:HD12	0.53	2.02	4	1
1:A:71:ALA:HB3	1:A:92:LEU:HD23	0.53	1.78	8	1
1:A:26:PRO:HB2	1:A:27:ALA:HB2	0.53	1.81	2	15
1:A:111:VAL:HG23	1:A:113:VAL:HG23	0.53	1.79	17	3
1:A:65:SER:CB	1:A:69:THR:HG21	0.53	2.33	10	1
1:A:48:LEU:HD22	1:A:48:LEU:C	0.53	2.29	17	1
1:A:69:THR:HG21	1:A:101:PHE:CG	0.52	2.39	1	1
1:A:69:THR:O	1:A:92:LEU:HD22	0.52	2.05	3	2
1:A:33:GLU:CD	1:A:126:VAL:HG12	0.51	2.30	15	1
1:A:31:VAL:CG2	1:A:41:VAL:HG23	0.50	2.36	18	1
1:A:32:ALA:HB1	1:A:126:VAL:HG21	0.50	1.84	3	2
1:A:69:THR:HG22	1:A:101:PHE:CD1	0.50	2.41	8	1
1:A:100:ILE:H	1:A:100:ILE:HD13	0.50	1.67	12	4
1:A:100:ILE:HG22	1:A:122:GLN:HG2	0.49	1.83	3	7
1:A:22:LEU:HD23	1:A:23:ILE:O	0.49	2.07	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HD11	1:A:74:VAL:HG13	0.49	1.83	16	1
1:A:20:LEU:HD13	1:A:21:HIS:N	0.49	2.21	16	2
1:A:62:ILE:HG23	1:A:103:LEU:HD21	0.49	1.84	7	3
1:A:111:VAL:HG13	1:A:113:VAL:HG23	0.49	1.83	9	2
1:A:56:ILE:C	1:A:56:ILE:HD12	0.48	2.33	11	1
1:A:92:LEU:HD13	1:A:93:ASP:N	0.48	2.24	10	1
1:A:33:GLU:OE1	1:A:126:VAL:HG12	0.48	2.09	15	1
1:A:119:LEU:HD13	1:A:119:LEU:C	0.48	2.33	17	1
1:A:100:ILE:O	1:A:100:ILE:HD12	0.48	2.09	4	1
1:A:106:TYR:CD1	1:A:116:LEU:HD12	0.48	2.43	13	1
1:A:119:LEU:HD23	1:A:119:LEU:C	0.48	2.34	4	9
1:A:22:LEU:H	1:A:22:LEU:HD22	0.48	1.69	16	2
1:A:34:ASN:HD21	1:A:71:ALA:HB3	0.48	1.68	17	1
1:A:99:ASN:OD1	1:A:100:ILE:HG23	0.48	2.09	9	3
1:A:56:ILE:C	1:A:56:ILE:HD13	0.47	2.34	6	1
1:A:65:SER:OG	1:A:69:THR:HG21	0.47	2.10	5	1
1:A:48:LEU:HD13	1:A:49:SER:N	0.47	2.25	16	1
1:A:56:ILE:HD12	1:A:56:ILE:N	0.47	2.24	16	1
1:A:77:LEU:HD23	1:A:83:GLU:OE2	0.47	2.09	2	1
1:A:33:GLU:CB	1:A:126:VAL:HG13	0.46	2.41	8	1
1:A:22:LEU:HD12	1:A:46:VAL:HG13	0.46	1.87	16	2
1:A:64:ASN:O	1:A:103:LEU:HD12	0.46	2.11	12	1
1:A:22:LEU:N	1:A:22:LEU:HD12	0.45	2.25	8	1
1:A:25:LEU:N	1:A:25:LEU:HD23	0.45	2.27	10	1
1:A:116:LEU:C	1:A:116:LEU:HD23	0.45	2.37	13	9
1:A:25:LEU:C	1:A:25:LEU:HD23	0.45	2.37	3	2
1:A:106:TYR:CE1	1:A:114:THR:HG23	0.45	2.47	18	1
1:A:77:LEU:HD23	1:A:77:LEU:C	0.45	2.37	17	4
1:A:62:ILE:HD12	1:A:62:ILE:N	0.44	2.27	10	2
1:A:68:LEU:CD2	1:A:92:LEU:HD12	0.44	2.42	16	1
1:A:22:LEU:HG	1:A:46:VAL:HG12	0.44	1.89	19	1
1:A:68:LEU:CD1	1:A:96:THR:HG22	0.44	2.42	2	1
1:A:48:LEU:HD22	1:A:80:THR:HG21	0.44	1.89	15	1
1:A:68:LEU:C	1:A:68:LEU:HD23	0.44	2.38	14	1
1:A:22:LEU:HD22	1:A:22:LEU:N	0.44	2.27	16	1
1:A:23:ILE:HD12	1:A:23:ILE:H	0.44	1.73	5	2
1:A:23:ILE:HD11	1:A:47:LYS:HG2	0.44	1.88	18	1
1:A:71:ALA:HB3	1:A:88:GLY:H	0.43	1.72	5	1
1:A:103:LEU:HD12	1:A:103:LEU:N	0.43	2.29	16	1
1:A:92:LEU:HD23	1:A:92:LEU:C	0.43	2.38	4	2
1:A:69:THR:HG22	1:A:101:PHE:CG	0.43	2.47	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:HD13	1:A:57:PRO:N	0.43	2.28	6	1
1:A:104:GLN:NE2	1:A:118:VAL:HG22	0.43	2.29	8	2
1:A:46:VAL:HG23	1:A:82:PHE:CE2	0.43	2.48	10	1
1:A:101:PHE:CD1	1:A:103:LEU:HD11	0.43	2.48	16	2
1:A:68:LEU:HD22	1:A:96:THR:HG22	0.43	1.90	11	1
1:A:48:LEU:HD23	1:A:80:THR:CG2	0.43	2.44	10	1
1:A:70:GLU:O	1:A:92:LEU:HD21	0.43	2.13	18	1
1:A:69:THR:HG23	1:A:101:PHE:CD1	0.42	2.47	12	1
1:A:77:LEU:C	1:A:77:LEU:HD23	0.42	2.40	5	1
1:A:85:VAL:HG12	1:A:87:THR:HG23	0.42	1.91	12	1
1:A:72:PHE:CE1	1:A:84:VAL:HG11	0.42	2.49	8	1
1:A:61:GLN:N	1:A:106:TYR:O	0.41	2.53	20	5
1:A:71:ALA:HB1	1:A:87:THR:HA	0.41	1.91	7	1
1:A:52:LEU:C	1:A:52:LEU:HD12	0.41	2.40	14	1
1:A:59:PHE:CZ	1:A:107:VAL:HG13	0.41	2.49	14	1
1:A:62:ILE:HD13	1:A:74:VAL:CG2	0.41	2.46	19	1
1:A:41:VAL:CG1	1:A:86:THR:HG23	0.41	2.46	10	1
1:A:22:LEU:CD1	1:A:46:VAL:HG13	0.41	2.46	16	1
1:A:31:VAL:HG11	1:A:41:VAL:HG22	0.41	1.91	20	1
1:A:116:LEU:HD23	1:A:116:LEU:C	0.41	2.41	5	1
1:A:48:LEU:O	1:A:48:LEU:HD12	0.41	2.16	9	1
1:A:105:ILE:HD12	1:A:105:ILE:N	0.41	2.30	10	1
1:A:22:LEU:HD12	1:A:22:LEU:N	0.41	2.31	14	1
1:A:22:LEU:HD12	1:A:46:VAL:HG22	0.41	1.93	15	1
1:A:106:TYR:OH	1:A:114:THR:HG22	0.41	2.16	11	2
1:A:25:LEU:HD12	1:A:25:LEU:N	0.40	2.31	6	1
1:A:69:THR:HG23	1:A:69:THR:O	0.40	2.16	9	1
1:A:119:LEU:C	1:A:119:LEU:HD23	0.40	2.41	13	1
1:A:104:GLN:HE22	1:A:118:VAL:HG22	0.40	1.76	10	1
1:A:44:PHE:CE2	1:A:119:LEU:HD12	0.40	2.51	20	1
1:A:70:GLU:O	1:A:71:ALA:HB2	0.40	2.17	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/126 (85%)	97±2 (91±2%)	7±2 (7±2%)	3±1 (3±1%)	6	43
All	All	2140/2520 (85%)	1940 (91%)	146 (7%)	54 (3%)	6	43

All 8 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	79	GLY	20
1	A	24	LEU	14
1	A	33	GLU	9
1	A	71	ALA	4
1	A	87	THR	4
1	A	88	GLY	1
1	A	36	PRO	1
1	A	52	LEU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	96/112 (86%)	92±2 (96±2%)	4±2 (4±2%)	29	79
All	All	1920/2240 (86%)	1844 (96%)	76 (4%)	29	79

All 31 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	24	LEU	10
1	A	52	LEU	8
1	A	106	TYR	6
1	A	22	LEU	5
1	A	61	GLN	4
1	A	100	ILE	4
1	A	33	GLU	3
1	A	43	LYS	3
1	A	119	LEU	3
1	A	44	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	48	LEU	3
1	A	56	ILE	2
1	A	77	LEU	2
1	A	95	GLU	2
1	A	20	LEU	2
1	A	105	ILE	1
1	A	117	GLN	1
1	A	107	VAL	1
1	A	92	LEU	1
1	A	113	VAL	1
1	A	34	ASN	1
1	A	90	GLU	1
1	A	25	LEU	1
1	A	101	PHE	1
1	A	94	PHE	1
1	A	124	THR	1
1	A	47	LYS	1
1	A	68	LEU	1
1	A	62	ILE	1
1	A	45	SER	1
1	A	73	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1403
Number of shifts mapped to atoms	1403
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	124	0.04 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	115	-0.09 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	121	-0.34 ± 0.11	None needed (< 0.5 ppm)
^{15}N	112	0.06 ± 0.54	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1227 atoms were assigned a chemical shift out of a possible 1427. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	516/526 (98%)	210/213 (99%)	209/214 (98%)	97/99 (98%)
Sidechain	709/797 (89%)	489/526 (93%)	220/254 (87%)	0/17 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	2/104 (2%)	1/52 (2%)	0/49 (0%)	1/3 (33%)
Overall	1227/1427 (86%)	700/791 (88%)	429/517 (83%)	98/119 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1403 atoms were assigned a chemical shift out of a possible 1646. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	603/619 (97%)	246/251 (98%)	245/252 (97%)	112/116 (97%)
Sidechain	798/914 (87%)	550/598 (92%)	248/295 (84%)	0/21 (0%)
Aromatic	2/113 (2%)	1/56 (2%)	0/54 (0%)	1/3 (33%)
Overall	1403/1646 (85%)	797/905 (88%)	493/601 (82%)	113/140 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

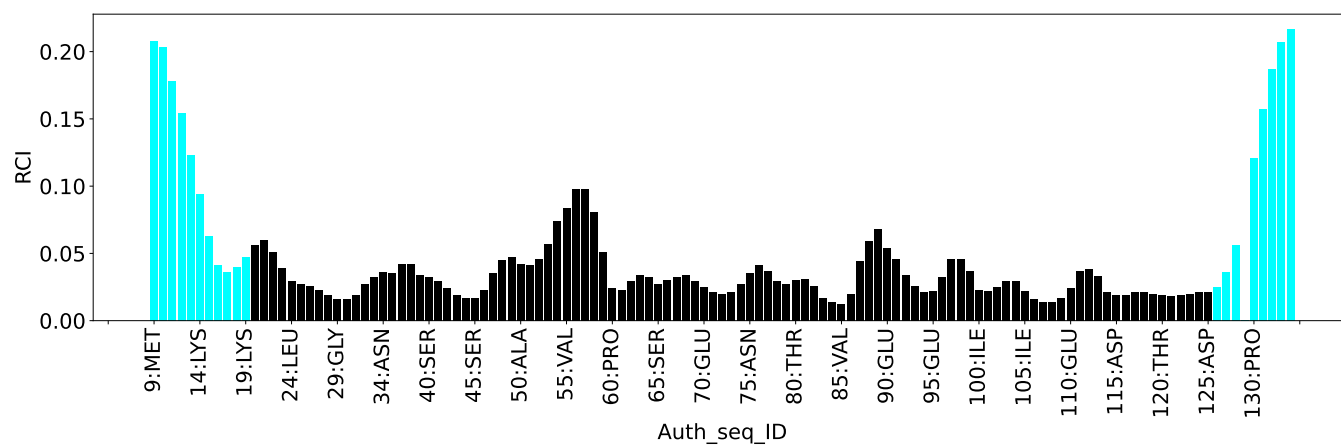
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	82	PHE	HB3	0.81	1.03 – 4.85	-5.6
1	A	129	PRO	HD2	1.89	1.93 – 5.38	-5.1

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	2081
Intra-residue ($ i-j =0$)	630
Sequential ($ i-j =1$)	455
Medium range ($ i-j >1$ and $ i-j <5$)	131
Long range ($ i-j \geq 5$)	751
Inter-chain	0
Hydrogen bond restraints	101
Disulfide bond restraints	0
Total dihedral-angle restraints	211
Number of unmapped restraints	0
Number of restraints per residue	17.8
Number of long range restraints per residue ¹	6.6

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	28.3	0.2
0.2-0.5 (Medium)	7.7	0.5
>0.5 (Large)	1.2	1.15

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)	17.0	4.94
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

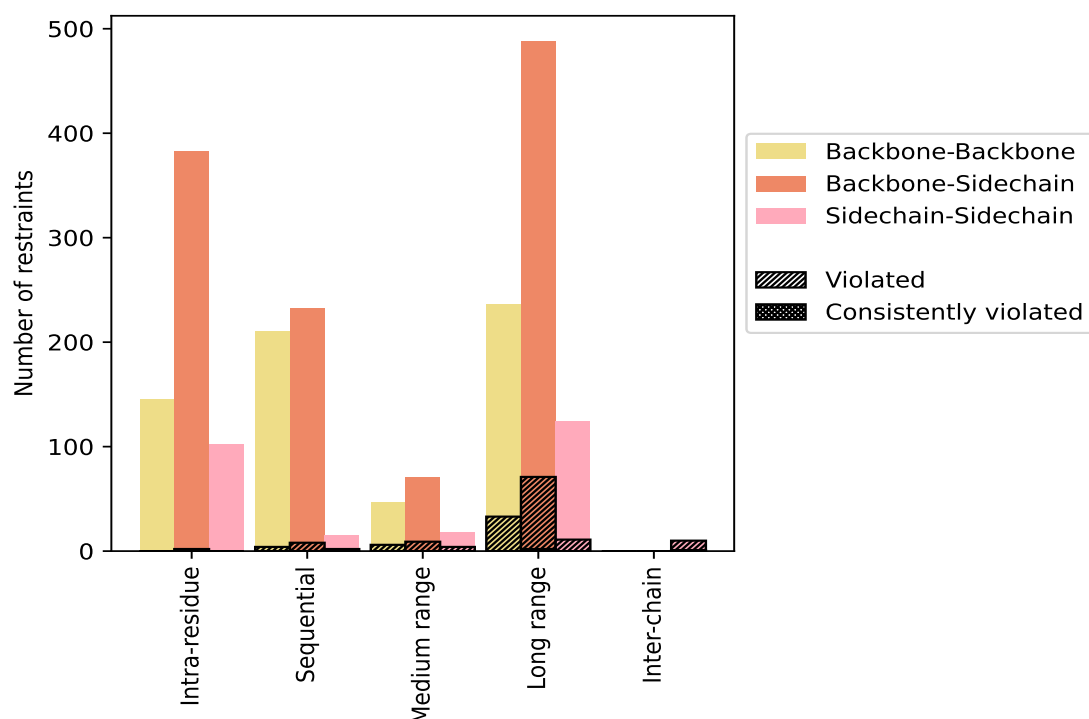
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	630	30.3	2	0.3	0.1	0	0.0	0.0
Backbone-Backbone	145	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	383	18.4	2	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	102	4.9	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	455	21.9	12	2.6	0.6	0	0.0	0.0
Backbone-Backbone	210	10.1	4	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	232	11.1	8	3.4	0.4	0	0.0	0.0
Sidechain-Sidechain	13	0.6	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	131	6.3	18	13.7	0.9	0	0.0	0.0
Backbone-Backbone	47	2.3	6	12.8	0.3	0	0.0	0.0
Backbone-Sidechain	67	3.2	9	13.4	0.4	0	0.0	0.0
Sidechain-Sidechain	17	0.8	3	17.6	0.1	0	0.0	0.0
Long range ($ i-j \geq 5$)	751	36.1	102	13.6	4.9	1	0.1	0.0
Backbone-Backbone	236	11.3	33	14.0	1.6	0	0.0	0.0
Backbone-Sidechain	391	18.8	58	14.8	2.8	1	0.3	0.0
Sidechain-Sidechain	124	6.0	11	8.9	0.5	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	101	4.9	13	12.9	0.6	1	1.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2081	100.0	160	7.7	7.7	3	0.1	0.1
Backbone-Backbone	638	30.7	43	6.7	2.1	0	0.0	0.0
Backbone-Sidechain	1174	56.4	90	7.7	4.3	2	0.2	0.1
Sidechain-Sidechain	269	12.9	27	10.0	1.3	1	0.4	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	4	3	24	7	38	0.18	0.41	0.07	0.16
2	0	6	2	31	3	42	0.17	0.51	0.08	0.15
3	0	4	2	27	6	39	0.21	1.15	0.19	0.14
4	1	5	2	24	6	38	0.24	0.88	0.19	0.16
5	0	6	1	27	6	40	0.18	0.58	0.1	0.15
6	0	4	2	33	8	47	0.21	1.02	0.16	0.16
7	0	2	3	27	3	35	0.16	0.31	0.05	0.15
8	0	3	3	23	7	36	0.2	0.7	0.13	0.16
9	0	4	2	31	2	39	0.16	0.31	0.06	0.14
10	0	4	3	26	6	39	0.17	0.39	0.06	0.15

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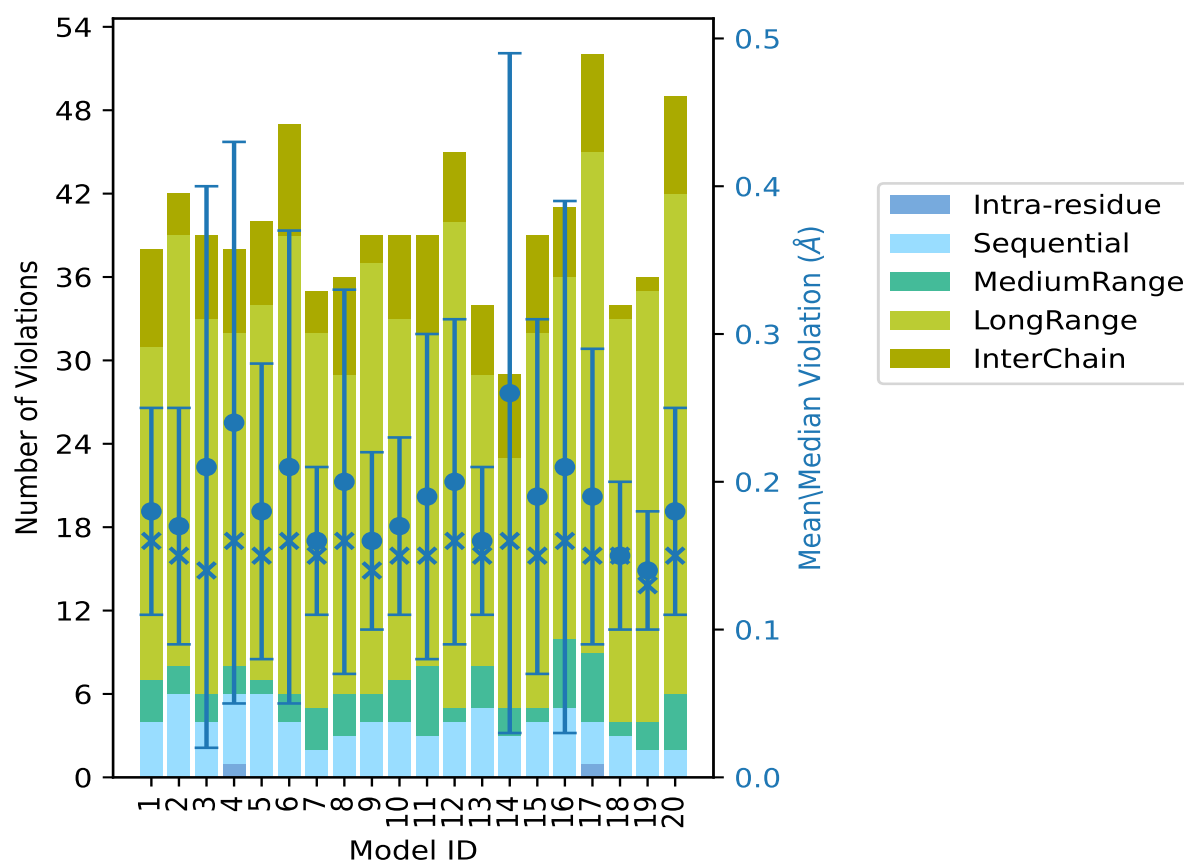
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	3	5	24	7	39	0.19	0.65	0.11	0.15
12	0	4	1	35	5	45	0.2	0.72	0.11	0.16
13	0	5	3	21	5	34	0.16	0.28	0.05	0.15
14	0	3	2	18	6	29	0.26	1.1	0.23	0.16
15	0	4	1	27	7	39	0.19	0.64	0.12	0.15
16	0	5	5	26	5	41	0.21	1.1	0.18	0.16
17	1	3	5	36	7	52	0.19	0.56	0.1	0.15
18	0	3	1	29	1	34	0.15	0.35	0.05	0.15
19	0	2	2	31	1	36	0.14	0.24	0.04	0.13
20	0	2	4	36	7	49	0.18	0.38	0.07	0.15

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

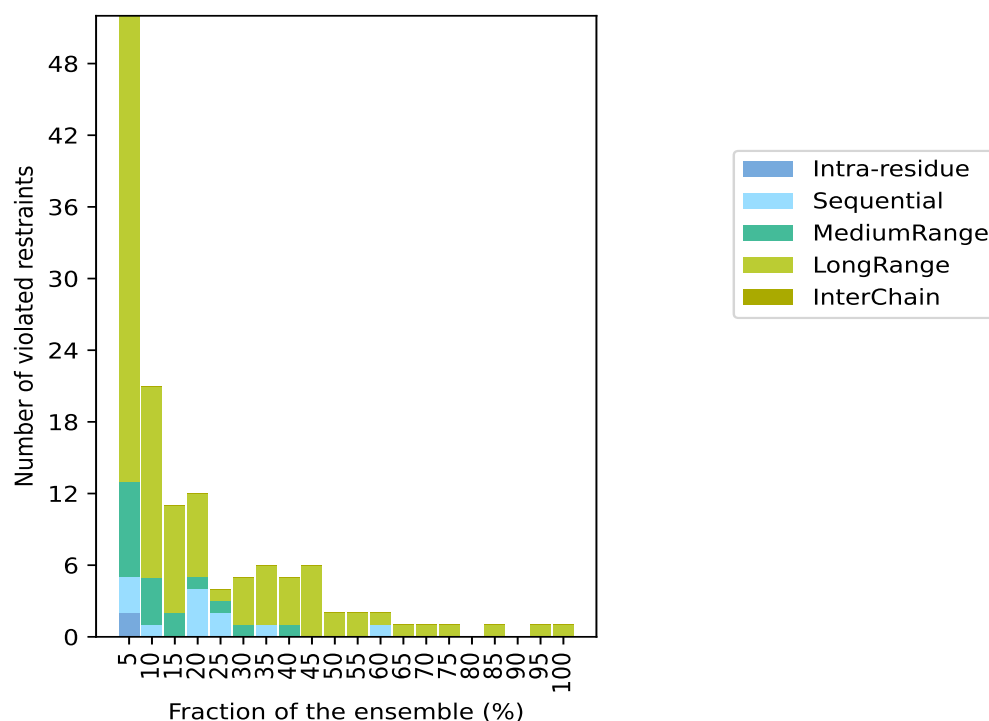
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1833(IR:628, SQ:443, MR:113, LR:649, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	3	8	39	0	52	1	5.0
0	1	4	16	0	21	2	10.0
0	0	2	9	0	11	3	15.0
0	4	1	7	0	12	4	20.0
0	2	1	1	0	4	5	25.0
0	0	1	4	0	5	6	30.0
0	1	0	5	0	6	7	35.0
0	0	1	4	0	5	8	40.0
0	0	0	6	0	6	9	45.0
0	0	0	2	0	2	10	50.0
0	0	0	2	0	2	11	55.0
0	1	0	1	0	2	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	1	0	1	20	100.0

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

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

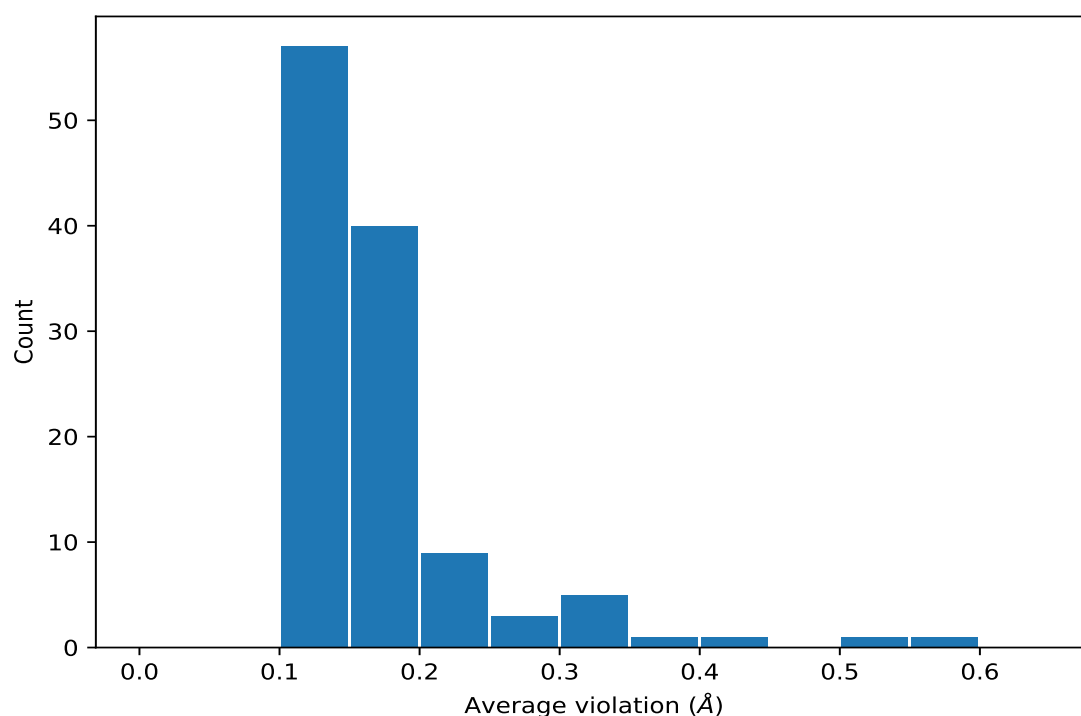
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	20	0.24	0.03	0.24
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	20	0.23	0.04	0.24
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	20	0.19	0.05	0.17
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	19	0.2	0.21	0.15
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	19	0.2	0.21	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	19	0.15	0.01	0.15
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	17	0.16	0.03	0.15
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	17	0.16	0.03	0.15
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	16	0.35	0.15	0.33
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	16	0.14	0.03	0.14
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	15	0.17	0.05	0.17
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	15	0.12	0.02	0.12
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	14	0.14	0.03	0.14
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	14	0.13	0.03	0.13
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	14	0.13	0.02	0.12
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	13	0.52	0.19	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	13	0.35	0.19	0.3
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	13	0.15	0.03	0.15
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	12	0.4	0.18	0.38
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	12	0.18	0.04	0.18
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	12	0.14	0.03	0.14
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	11	0.39	0.22	0.34
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	11	0.15	0.04	0.15
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	11	0.14	0.03	0.14
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	10	0.32	0.16	0.28
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	10	0.17	0.04	0.18
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	10	0.16	0.06	0.15
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	10	0.13	0.03	0.12
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	9	0.18	0.05	0.15
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	9	0.15	0.03	0.14
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	9	0.15	0.03	0.14
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	9	0.14	0.01	0.14
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	9	0.14	0.05	0.12
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	9	0.12	0.01	0.12
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	8	0.59	0.37	0.4
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	8	0.19	0.06	0.2
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	8	0.16	0.02	0.15
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	8	0.15	0.04	0.14
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	8	0.14	0.03	0.12
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	8	0.13	0.02	0.14
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	7	0.34	0.1	0.29
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	7	0.23	0.05	0.23
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	7	0.21	0.13	0.15
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	7	0.19	0.04	0.19
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	7	0.17	0.03	0.15
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	7	0.16	0.03	0.16
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	7	0.15	0.05	0.13
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	7	0.15	0.05	0.15
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	7	0.14	0.03	0.14
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	7	0.13	0.02	0.12
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	7	0.12	0.01	0.13
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	7	0.12	0.02	0.12
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	6	0.18	0.04	0.16
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	6	0.17	0.07	0.16
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	6	0.16	0.04	0.15
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	6	0.16	0.03	0.16
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	6	0.16	0.03	0.16
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	6	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	6	0.13	0.03	0.12
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	5	0.19	0.04	0.18
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	5	0.18	0.08	0.15
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	5	0.15	0.01	0.15
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	5	0.11	0.01	0.11
(3,671)	1:51:A:SER:H	1:52:A:LEU:HB3	4	0.33	0.06	0.34
(3,413)	1:34:A:ASN:H	1:126:A:VAL:H	4	0.2	0.04	0.18
(3,651)	1:48:A:LEU:HG	1:49:A:SER:H	4	0.19	0.06	0.17
(3,849)	1:62:A:ILE:HB	1:73:A:ARG:HA	4	0.18	0.07	0.16
(3,1427)	1:97:A:GLY:H	1:98:A:PRO:HA	4	0.18	0.03	0.18
(3,1430)	1:97:A:GLY:HA2	1:98:A:PRO:HA	4	0.17	0.04	0.16
(3,1087)	1:72:A:PHE:H	1:86:A:THR:HA	4	0.16	0.01	0.16
(1,9)	2:203:A:CA:CA	1:126:A:VAL:O	4	0.16	0.02	0.16
(3,353)	1:31:A:VAL:HG11	1:35:A:SER:H	4	0.15	0.02	0.15
(3,353)	1:31:A:VAL:HG12	1:35:A:SER:H	4	0.15	0.02	0.15
(3,353)	1:31:A:VAL:HG13	1:35:A:SER:H	4	0.15	0.02	0.15
(3,300)	1:29:A:GLY:HA2	1:121:A:VAL:H	4	0.14	0.03	0.14
(3,1639)	1:107:A:VAL:H	1:114:A:THR:HB	4	0.14	0.03	0.14
(3,1652)	1:107:A:VAL:H	1:115:A:ASP:HA	4	0.13	0.02	0.13
(3,938)	1:64:A:ASN:H	1:105:A:ILE:H	4	0.11	0.01	0.11
(3,190)	1:23:A:ILE:HD11	1:46:A:VAL:H	3	0.26	0.07	0.25
(3,190)	1:23:A:ILE:HD12	1:46:A:VAL:H	3	0.26	0.07	0.25
(3,190)	1:23:A:ILE:HD13	1:46:A:VAL:H	3	0.26	0.07	0.25
(3,582)	1:44:A:PHE:H	1:82:A:PHE:HB3	3	0.2	0.07	0.24
(3,407)	1:33:A:GLU:HA	1:124:A:THR:HB	3	0.16	0.01	0.16
(3,34)	1:13:A:TYR:HB3	1:15:A:ASP:H	3	0.16	0.03	0.18
(3,449)	1:38:A:GLY:H	1:86:A:THR:HB	3	0.16	0.02	0.16
(3,1224)	1:77:A:LEU:H	1:80:A:THR:H	3	0.16	0.01	0.15
(3,1186)	1:75:A:ASN:H	1:82:A:PHE:HA	3	0.15	0.02	0.16
(3,143)	1:22:A:LEU:HA	1:47:A:LYS:HA	3	0.14	0.0	0.14
(3,1589)	1:105:A:ILE:HD11	1:119:A:LEU:HG	3	0.14	0.02	0.14
(3,1589)	1:105:A:ILE:HD12	1:119:A:LEU:HG	3	0.14	0.02	0.14
(3,1589)	1:105:A:ILE:HD13	1:119:A:LEU:HG	3	0.14	0.02	0.14
(3,1486)	1:101:A:PHE:HB2	1:121:A:VAL:H	3	0.11	0.0	0.11
(3,822)	1:61:A:GLN:HA	1:74:A:VAL:HB	3	0.1	0.0	0.1
(3,1071)	1:72:A:PHE:HB2	1:74:A:VAL:H	2	0.21	0.06	0.21
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB2	2	0.18	0.04	0.18
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB3	2	0.18	0.04	0.18
(3,1406)	1:94:A:PHE:HA	1:99:A:ASN:HA	2	0.18	0.05	0.18
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB2	2	0.17	0.03	0.17
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB3	2	0.17	0.03	0.17
(3,611)	1:46:A:VAL:HB	1:81:A:TYR:HA	2	0.16	0.04	0.16

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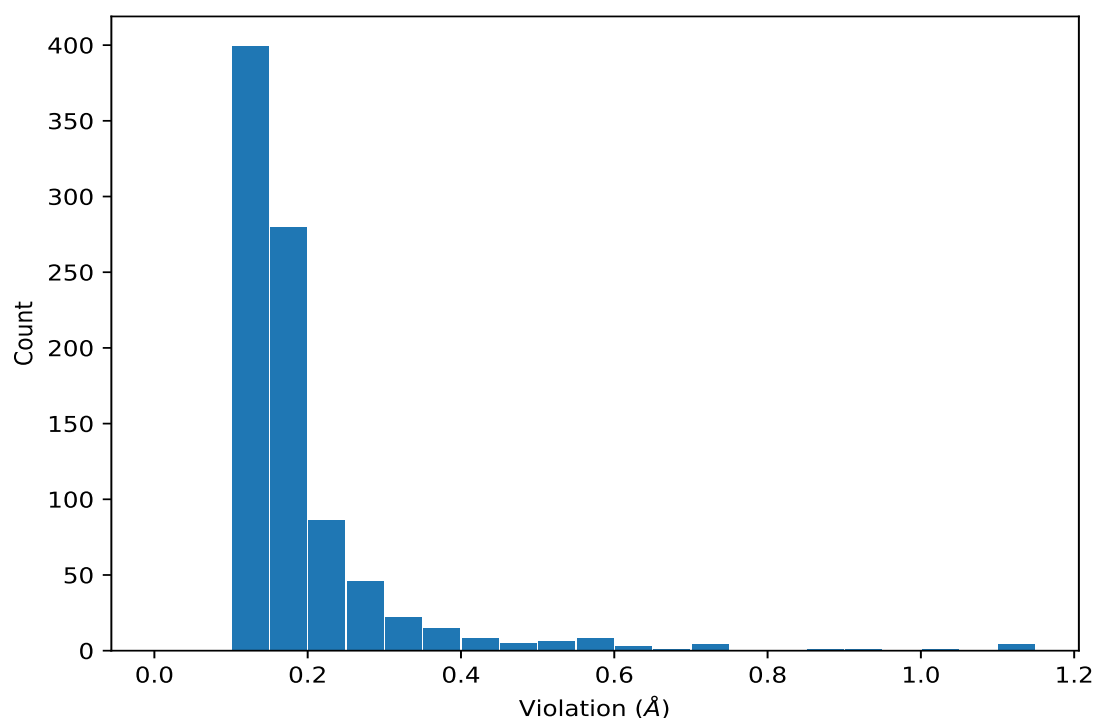
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG21	2	0.16	0.02	0.16
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG22	2	0.16	0.02	0.16
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG23	2	0.16	0.02	0.16
(3,1599)	1:105:A:ILE:HB	1:119:A:LEU:H	2	0.16	0.05	0.16
(3,1099)	1:73:A:ARG:H	1:75:A:ASN:H	2	0.15	0.01	0.15
(3,927)	1:64:A:ASN:HB2	1:103:A:LEU:HA	2	0.14	0.04	0.14
(3,989)	1:66:A:ASN:H	1:103:A:LEU:H	2	0.14	0.04	0.14
(3,1064)	1:71:A:ALA:HA	1:87:A:THR:H	2	0.14	0.02	0.14
(3,1418)	1:95:A:GLU:HA	1:97:A:GLY:H	2	0.14	0.01	0.14
(3,704)	1:53:A:SER:H	1:110:A:GLU:H	2	0.13	0.02	0.13
(3,1036)	1:70:A:GLU:HA	1:90:A:GLU:HA	2	0.13	0.02	0.13
(3,1498)	1:102:A:ASP:HB2	1:120:A:THR:H	2	0.12	0.01	0.12
(3,1452)	1:100:A:ILE:HB	1:102:A:ASP:HA	2	0.12	0.02	0.12
(3,603)	1:45:A:SER:H	1:81:A:TYR:HA	2	0.12	0.0	0.12
(3,1606)	1:105:A:ILE:H	1:116:A:LEU:HA	2	0.12	0.0	0.12
(3,116)	1:21:A:HIS:HA	1:115:A:ASP:HB3	2	0.11	0.0	0.11
(3,868)	1:62:A:ILE:H	1:105:A:ILE:HA	2	0.11	0.0	0.11
(3,1653)	1:107:A:VAL:H	1:114:A:THR:HA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	3	1.15
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	14	1.1
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	14	1.1
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	16	1.1
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	6	1.02
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	14	0.91
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	4	0.88
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	4	0.74
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	12	0.72
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	8	0.7
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	16	0.7
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	11	0.65
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	15	0.64
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	4	0.63
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	14	0.63
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	6	0.59
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	5	0.58
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	8	0.57
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	4	0.57
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	17	0.56
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	3	0.56
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	4	0.55
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	2	0.51
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	11	0.51
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	14	0.51
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	3	0.5
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	6	0.5
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	16	0.5
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	12	0.47
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	15	0.47
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	15	0.46
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	2	0.45
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	4	0.45
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	6	0.44
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	17	0.43
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	5	0.42
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	16	0.42
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	8	0.42
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	1	0.41
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	17	0.4
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	17	0.4
(3,671)	1:51:A:SER:H	1:52:A:LEU:HB3	15	0.39
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	17	0.39
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	10	0.39
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	11	0.38
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	20	0.38
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	4	0.37
(3,671)	1:51:A:SER:H	1:52:A:LEU:HB3	4	0.36
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	5	0.36
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	6	0.36
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	8	0.36
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	10	0.36
(3,190)	1:23:A:ILE:HD11	1:46:A:VAL:H	18	0.35
(3,190)	1:23:A:ILE:HD12	1:46:A:VAL:H	18	0.35
(3,190)	1:23:A:ILE:HD13	1:46:A:VAL:H	18	0.35
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	17	0.35
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	8	0.34
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	15	0.34
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	20	0.34
(3,671)	1:51:A:SER:H	1:52:A:LEU:HB3	6	0.33
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	20	0.33
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	1	0.33
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	6	0.32
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	1	0.32
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	5	0.32
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	6	0.32
(1,1)	2:201:A:CA:CA	1:33:A:GLU:OE1	20	0.32
(3,1638)	1:107:A:VAL:HB	1:115:A:ASP:HA	9	0.31
(3,963)	1:65:A:SER:HB2	1:101:A:PHE:HB3	5	0.31
(3,963)	1:65:A:SER:HB3	1:101:A:PHE:HB3	5	0.31
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	8	0.31
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	7	0.31
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	12	0.31
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	20	0.3
(3,849)	1:62:A:ILE:HB	1:73:A:ARG:HA	11	0.3
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	12	0.3
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	12	0.3
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	2	0.29
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	20	0.29
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	1	0.29
(3,651)	1:48:A:LEU:HG	1:49:A:SER:H	17	0.29
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	7	0.29
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	11	0.29
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	15	0.29
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	12	0.28
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	16	0.28
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	17	0.28
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	2	0.28
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	9	0.28
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	13	0.28
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	9	0.27
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	6	0.27
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	10	0.27
(3,1182)	1:75:A:ASN:H	1:82:A:PHE:HB2	17	0.27
(3,1071)	1:72:A:PHE:HB2	1:74:A:VAL:H	11	0.27
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	1	0.27
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	6	0.27
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	9	0.26
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	13	0.26
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	15	0.26
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	17	0.26
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	12	0.26
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	2	0.26
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	12	0.26
(3,582)	1:44:A:PHE:H	1:82:A:PHE:HB3	20	0.26
(3,413)	1:34:A:ASN:H	1:126:A:VAL:H	16	0.26
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	20	0.26
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	3	0.26
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	5	0.25
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	7	0.25
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	16	0.25
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	12	0.25
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	3	0.25
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	3	0.25
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	5	0.25
(3,190)	1:23:A:ILE:HD11	1:46:A:VAL:H	4	0.25
(3,190)	1:23:A:ILE:HD12	1:46:A:VAL:H	4	0.25
(3,190)	1:23:A:ILE:HD13	1:46:A:VAL:H	4	0.25
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	20	0.25
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	10	0.25
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	14	0.25
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	9	0.25
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	4	0.24
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	9	0.24
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	14	0.24
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	12	0.24
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	19	0.24
(3,1406)	1:94:A:PHE:HA	1:99:A:ASN:HA	12	0.24
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	9	0.24
(3,582)	1:44:A:PHE:H	1:82:A:PHE:HB3	15	0.24
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	13	0.24
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	13	0.24
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	1	0.24
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	7	0.24
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	15	0.24
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	8	0.23
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	17	0.23
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	14	0.23
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	12	0.23
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	3	0.23
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	4	0.23
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	8	0.23
(3,1430)	1:97:A:GLY:HA2	1:98:A:PRO:HA	3	0.23
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	15	0.23
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	6	0.23
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	9	0.23
(3,671)	1:51:A:SER:H	1:52:A:LEU:HB3	5	0.23
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	10	0.23
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	20	0.23
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	13	0.23
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	12	0.23
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	18	0.22
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	14	0.22
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	19	0.22
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	9	0.22
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	18	0.22
(3,1427)	1:97:A:GLY:H	1:98:A:PRO:HA	16	0.22
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	10	0.22
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	7	0.22
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	20	0.22
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB2	10	0.22
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB3	10	0.22
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	1	0.22
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	16	0.22
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	1	0.22
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	5	0.22
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	2	0.22
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	1	0.21
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	13	0.21
(3,1599)	1:105:A:ILE:HB	1:119:A:LEU:H	14	0.21
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	18	0.21
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	14	0.21
(3,1051)	1:70:A:GLU:H	1:70:A:GLU:HG2	17	0.21
(3,1034)	1:69:A:THR:HB	1:101:A:PHE:HB2	16	0.21
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	1	0.21
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	1	0.21
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	7	0.21
(3,611)	1:46:A:VAL:HB	1:81:A:TYR:HA	8	0.21
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	12	0.21
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	13	0.21
(1,8)	2:202:A:CA:CA	1:95:A:GLU:OE2	20	0.21
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	8	0.2
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	10	0.2
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	19	0.2
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	20	0.2
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	10	0.2
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	20	0.2
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	2	0.2
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	7	0.2
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	19	0.2
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	2	0.2
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	18	0.2
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	15	0.2
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	1	0.2
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	1	0.2
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	15	0.2
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	15	0.2
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	8	0.2
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	8	0.2
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	11	0.2
(3,413)	1:34:A:ASN:H	1:126:A:VAL:H	12	0.2
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB2	12	0.2
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB3	12	0.2
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	10	0.2
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	10	0.2
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	11	0.2
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	19	0.19
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	10	0.19
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	5	0.19
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	11	0.19
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	5	0.19
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	11	0.19
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	3	0.19
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	1	0.19
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	10	0.19
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	11	0.19
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	2	0.19
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	2	0.19
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	6	0.19
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	6	0.19
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	15	0.19
(3,651)	1:48:A:LEU:HG	1:49:A:SER:H	5	0.19
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	6	0.19
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	2	0.19
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	3	0.19
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	16	0.19
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	16	0.19
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	16	0.19
(3,353)	1:31:A:VAL:HG11	1:35:A:SER:H	1	0.19
(3,353)	1:31:A:VAL:HG12	1:35:A:SER:H	1	0.19
(3,353)	1:31:A:VAL:HG13	1:35:A:SER:H	1	0.19
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	19	0.19
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	2	0.19
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	20	0.19
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	16	0.19
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	16	0.19
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	1	0.19
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	5	0.19
(1,7)	2:202:A:CA:CA	1:95:A:GLU:OE1	14	0.19
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	1	0.19
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	6	0.18
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	18	0.18
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG21	3	0.18
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG22	3	0.18
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG23	3	0.18
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	13	0.18
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	13	0.18
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	16	0.18
(3,1639)	1:107:A:VAL:H	1:114:A:THR:HB	18	0.18
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	11	0.18
(3,1485)	1:101:A:PHE:HB3	1:121:A:VAL:H	14	0.18
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	7	0.18
(3,1430)	1:97:A:GLY:HA2	1:98:A:PRO:HA	4	0.18
(3,1427)	1:97:A:GLY:H	1:98:A:PRO:HA	15	0.18
(3,1224)	1:77:A:LEU:H	1:80:A:THR:H	18	0.18
(3,1087)	1:72:A:PHE:H	1:86:A:THR:HA	5	0.18
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	9	0.18
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	9	0.18
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	4	0.18
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	13	0.18
(3,753)	1:56:A:ILE:H	1:110:A:GLU:HB3	18	0.18
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,597)	1:45:A:SER:HA	1:82:A:PHE:HB3	17	0.18
(3,449)	1:38:A:GLY:H	1:86:A:THR:HB	1	0.18
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	4	0.18
(3,407)	1:33:A:GLU:HA	1:124:A:THR:HB	8	0.18
(3,147)	1:22:A:LEU:HB2	1:46:A:VAL:HG11	17	0.18
(3,147)	1:22:A:LEU:HB2	1:46:A:VAL:HG12	17	0.18
(3,147)	1:22:A:LEU:HB2	1:46:A:VAL:HG13	17	0.18
(3,147)	1:22:A:LEU:HB3	1:46:A:VAL:HG11	17	0.18
(3,147)	1:22:A:LEU:HB3	1:46:A:VAL:HG12	17	0.18
(3,147)	1:22:A:LEU:HB3	1:46:A:VAL:HG13	17	0.18
(3,34)	1:13:A:TYR:HB3	1:15:A:ASP:H	11	0.18
(3,34)	1:13:A:TYR:HB3	1:15:A:ASP:H	17	0.18
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	12	0.18
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	3	0.18
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	20	0.18
(1,9)	2:203:A:CA:CA	1:126:A:VAL:O	13	0.18
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	2	0.18
(1,6)	2:202:A:CA:CA	1:33:A:GLU:OE2	6	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	1	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	2	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	6	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	8	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	10	0.18
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	19	0.18
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	8	0.18
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	8	0.17
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	6	0.17
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	2	0.17
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	17	0.17
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	12	0.17
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	19	0.17
(3,1427)	1:97:A:GLY:H	1:98:A:PRO:HA	6	0.17
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	12	0.17
(3,1132)	1:74:A:VAL:H	1:105:A:ILE:HD11	10	0.17
(3,1132)	1:74:A:VAL:H	1:105:A:ILE:HD12	10	0.17
(3,1132)	1:74:A:VAL:H	1:105:A:ILE:HD13	10	0.17
(3,1087)	1:72:A:PHE:H	1:86:A:THR:HA	3	0.17
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	7	0.17
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	7	0.17
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	8	0.17
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	8	0.17
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	12	0.17
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	16	0.17
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	16	0.17
(3,989)	1:66:A:ASN:H	1:103:A:LEU:H	3	0.17
(3,927)	1:64:A:ASN:HB2	1:103:A:LEU:HA	17	0.17
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	10	0.17
(3,849)	1:62:A:ILE:HB	1:73:A:ARG:HA	9	0.17
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	2	0.17
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	13	0.17
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	3	0.17
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	12	0.17
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	19	0.17
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	6	0.17
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	20	0.17
(3,413)	1:34:A:ASN:H	1:126:A:VAL:H	10	0.17
(3,300)	1:29:A:GLY:HA2	1:121:A:VAL:H	17	0.17
(3,190)	1:23:A:ILE:HD11	1:46:A:VAL:H	20	0.17
(3,190)	1:23:A:ILE:HD12	1:46:A:VAL:H	20	0.17
(3,190)	1:23:A:ILE:HD13	1:46:A:VAL:H	20	0.17
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	16	0.17
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	15	0.17
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	8	0.17
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	12	0.17
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	20	0.17
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	8	0.17
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	10	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	3	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	5	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	7	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	13	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	17	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	18	0.17
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	20	0.17
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	9	0.17
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	9	0.16
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	15	0.16
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	18	0.16
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	11	0.16
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	12	0.16
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	17	0.16
(3,1949)	1:133:A:THR:H	1:134:A:LYS:HA	18	0.16
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	4	0.16
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	14	0.16
(3,1639)	1:107:A:VAL:H	1:114:A:THR:HB	19	0.16
(3,1589)	1:105:A:ILE:HD11	1:119:A:LEU:HG	6	0.16
(3,1589)	1:105:A:ILE:HD12	1:119:A:LEU:HG	6	0.16
(3,1589)	1:105:A:ILE:HD13	1:119:A:LEU:HG	6	0.16
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	4	0.16
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	7	0.16
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	13	0.16
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	5	0.16
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	1	0.16
(3,1186)	1:75:A:ASN:H	1:82:A:PHE:HA	19	0.16
(3,1186)	1:75:A:ASN:H	1:82:A:PHE:HA	20	0.16
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	17	0.16
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	4	0.16
(3,1099)	1:73:A:ARG:H	1:75:A:ASN:H	16	0.16
(3,1087)	1:72:A:PHE:H	1:86:A:THR:HA	7	0.16
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	11	0.16
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	16	0.16
(3,1064)	1:71:A:ALA:HA	1:87:A:THR:H	6	0.16
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	9	0.16
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	9	0.16
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	16	0.16
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	16	0.16
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	17	0.16
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	17	0.16
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	6	0.16
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	13	0.16
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	10	0.16
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	8	0.16
(3,449)	1:38:A:GLY:H	1:86:A:THR:HB	18	0.16
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	4	0.16
(3,413)	1:34:A:ASN:H	1:126:A:VAL:H	17	0.16
(3,407)	1:33:A:GLU:HA	1:124:A:THR:HB	6	0.16
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	6	0.16
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	6	0.16
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	12	0.16
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	12	0.16
(3,353)	1:31:A:VAL:HG11	1:35:A:SER:H	7	0.16
(3,353)	1:31:A:VAL:HG12	1:35:A:SER:H	7	0.16
(3,353)	1:31:A:VAL:HG13	1:35:A:SER:H	7	0.16
(3,300)	1:29:A:GLY:HA2	1:121:A:VAL:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	2	0.16
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	5	0.16
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	10	0.16
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	12	0.16
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	11	0.16
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	3	0.16
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	14	0.16
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	20	0.16
(1,9)	2:203:A:CA:CA	1:126:A:VAL:O	1	0.16
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	20	0.16
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	15	0.16
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	16	0.16
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	18	0.15
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	7	0.15
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	5	0.15
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	3	0.15
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	2	0.15
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	12	0.15
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	14	0.15
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	16	0.15
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	18	0.15
(3,1652)	1:107:A:VAL:H	1:115:A:ASP:HA	2	0.15
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	10	0.15
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	15	0.15
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	16	0.15
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	18	0.15
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	7	0.15
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	15	0.15
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	16	0.15
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	20	0.15
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	12	0.15
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	16	0.15
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	18	0.15
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	20	0.15
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	2	0.15
(3,1430)	1:97:A:GLY:HA2	1:98:A:PRO:HA	1	0.15
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	19	0.15
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	20	0.15
(3,1224)	1:77:A:LEU:H	1:80:A:THR:H	1	0.15
(3,1224)	1:77:A:LEU:H	1:80:A:THR:H	9	0.15
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	10	0.15
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	10	0.15
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	11	0.15
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	16	0.15
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	17	0.15
(3,1087)	1:72:A:PHE:H	1:86:A:THR:HA	20	0.15
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	4	0.15
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	17	0.15
(3,1071)	1:72:A:PHE:HB2	1:74:A:VAL:H	8	0.15
(3,1059)	1:71:A:ALA:H	1:90:A:GLU:HB2	12	0.15
(3,1059)	1:71:A:ALA:H	1:90:A:GLU:HB3	12	0.15
(3,1036)	1:70:A:GLU:HA	1:90:A:GLU:HA	11	0.15
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	6	0.15
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	6	0.15
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	12	0.15
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	12	0.15
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	13	0.15
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	13	0.15
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	20	0.15
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	20	0.15
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	7	0.15
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	7	0.15
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	11	0.15
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	11	0.15
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	15	0.15
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	15	0.15
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	7	0.15
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	13	0.15
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	6	0.15
(3,849)	1:62:A:ILE:HB	1:73:A:ARG:HA	12	0.15
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB2	6	0.15
(3,810)	1:61:A:GLN:HA	1:106:A:TYR:HB3	6	0.15
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	7	0.15
(3,704)	1:53:A:SER:H	1:110:A:GLU:H	12	0.15
(3,651)	1:48:A:LEU:HG	1:49:A:SER:H	15	0.15
(3,632)	1:47:A:LYS:H	1:49:A:SER:H	10	0.15
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	12	0.15
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	20	0.15
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	16	0.15
(3,407)	1:33:A:GLU:HA	1:124:A:THR:HB	17	0.15
(3,357)	1:31:A:VAL:HA	1:124:A:THR:H	17	0.15
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	17	0.15
(3,143)	1:22:A:LEU:HA	1:47:A:LYS:HA	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	2	0.15
(3,140)	1:22:A:LEU:HG	1:47:A:LYS:H	16	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	4	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	6	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	9	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	16	0.15
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	18	0.15
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	5	0.15
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	7	0.15
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	16	0.15
(1,9)	2:203:A:CA:CA	1:126:A:VAL:O	17	0.15
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	11	0.15
(1,3)	2:201:A:CA:CA	1:125:A:ASP:OD1	14	0.15
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	7	0.14
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	11	0.14
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	14	0.14
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	16	0.14
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	17	0.14
(4,25)	1:46:A:VAL:H	1:80:A:THR:O	20	0.14
(4,15)	1:39:A:THR:O	1:86:A:THR:H	19	0.14
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	12	0.14
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	19	0.14
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	10	0.14
(4,1)	1:21:A:HIS:O	1:47:A:LYS:N	13	0.14
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	1	0.14
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	4	0.14
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG21	5	0.14
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG22	5	0.14
(3,1826)	1:117:A:GLN:HA	1:118:A:VAL:HG23	5	0.14
(3,1716)	1:109:A:ASP:HB3	1:113:A:VAL:HG21	11	0.14
(3,1716)	1:109:A:ASP:HB3	1:113:A:VAL:HG22	11	0.14
(3,1716)	1:109:A:ASP:HB3	1:113:A:VAL:HG23	11	0.14
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	20	0.14
(3,1652)	1:107:A:VAL:H	1:115:A:ASP:HA	20	0.14
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	5	0.14
(3,1637)	1:107:A:VAL:HG11	1:109:A:ASP:HA	9	0.14
(3,1637)	1:107:A:VAL:HG12	1:109:A:ASP:HA	9	0.14
(3,1637)	1:107:A:VAL:HG13	1:109:A:ASP:HA	9	0.14
(3,1589)	1:105:A:ILE:HD11	1:119:A:LEU:HG	15	0.14
(3,1589)	1:105:A:ILE:HD12	1:119:A:LEU:HG	15	0.14
(3,1589)	1:105:A:ILE:HD13	1:119:A:LEU:HG	15	0.14
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	18	0.14
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	2	0.14
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	8	0.14
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	15	0.14
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	9	0.14
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	19	0.14
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	2	0.14
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	17	0.14
(3,1452)	1:100:A:ILE:HB	1:102:A:ASP:HA	3	0.14
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	17	0.14
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	9	0.14
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	12	0.14
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	15	0.14
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	16	0.14
(3,1418)	1:95:A:GLU:HA	1:97:A:GLY:H	7	0.14
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	9	0.14
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	9	0.14
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	1	0.14
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	10	0.14
(3,1099)	1:73:A:ARG:H	1:75:A:ASN:H	4	0.14
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	2	0.14
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	9	0.14
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	10	0.14
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	20	0.14
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	4	0.14
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	4	0.14
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	17	0.14
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	17	0.14
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	18	0.14
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	18	0.14
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	4	0.14
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	4	0.14
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	18	0.14
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	18	0.14
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	19	0.14
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	19	0.14
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	20	0.14
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	3	0.14
(3,806)	1:61:A:GLN:HA	1:105:A:ILE:HG21	20	0.14
(3,806)	1:61:A:GLN:HA	1:105:A:ILE:HG22	20	0.14
(3,806)	1:61:A:GLN:HA	1:105:A:ILE:HG23	20	0.14
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,651)	1:48:A:LEU:HG	1:49:A:SER:H	13	0.14
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	8	0.14
(3,449)	1:38:A:GLY:H	1:86:A:THR:HB	19	0.14
(3,417)	1:35:A:SER:H	1:92:A:LEU:H	6	0.14
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB2	13	0.14
(3,410)	1:34:A:ASN:HA	1:92:A:LEU:HB3	13	0.14
(3,316)	1:29:A:GLY:HA2	1:122:A:GLN:H	5	0.14
(3,143)	1:22:A:LEU:HA	1:47:A:LYS:HA	3	0.14
(3,143)	1:22:A:LEU:HA	1:47:A:LYS:HA	6	0.14
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	4	0.14
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	10	0.14
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	12	0.14
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	14	0.14
(3,126)	1:21:A:HIS:H	1:47:A:LYS:HD2	9	0.14
(3,126)	1:21:A:HIS:H	1:47:A:LYS:HD3	9	0.14
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	2	0.14
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	4	0.14
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	11	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	1	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	7	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	8	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	11	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	13	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	14	0.14
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	17	0.14
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	4	0.14
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	9	0.14
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	14	0.14
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	10	0.14
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	13	0.14
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	10	0.14
(4,29)	1:61:A:GLN:H	1:106:A:TYR:O	3	0.13
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	1	0.13
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	4	0.13
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	16	0.13
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	20	0.13
(3,1832)	1:118:A:VAL:HB	1:120:A:THR:H	5	0.13
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	5	0.13
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	13	0.13
(3,1604)	1:105:A:ILE:H	1:119:A:LEU:HB2	17	0.13
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	1	0.13
(3,1539)	1:103:A:LEU:H	1:120:A:THR:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1498)	1:102:A:ASP:HB2	1:120:A:THR:H	14	0.13
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	5	0.13
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	6	0.13
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	3	0.13
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	14	0.13
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	4	0.13
(3,1427)	1:97:A:GLY:H	1:98:A:PRO:HA	12	0.13
(3,1418)	1:95:A:GLU:HA	1:97:A:GLY:H	16	0.13
(3,1406)	1:94:A:PHE:HA	1:99:A:ASN:HA	16	0.13
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	13	0.13
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	13	0.13
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	19	0.13
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	19	0.13
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	20	0.13
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	20	0.13
(3,981)	1:66:A:ASN:H	1:103:A:LEU:HG	12	0.13
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	6	0.13
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	8	0.13
(3,938)	1:64:A:ASN:H	1:105:A:ILE:H	2	0.13
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	5	0.13
(3,841)	1:62:A:ILE:HG13	1:105:A:ILE:HB	11	0.13
(3,798)	1:60:A:PRO:HB3	1:61:A:GLN:H	12	0.13
(3,730)	1:55:A:VAL:HA	1:110:A:GLU:HG2	5	0.13
(3,618)	1:46:A:VAL:HB	1:80:A:THR:HA	17	0.13
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	14	0.13
(3,504)	1:41:A:VAL:HA	1:86:A:THR:HG21	17	0.13
(3,504)	1:41:A:VAL:HA	1:86:A:THR:HG22	17	0.13
(3,504)	1:41:A:VAL:HA	1:86:A:THR:HG23	17	0.13
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	9	0.13
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	12	0.13
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	2	0.13
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	2	0.13
(3,353)	1:31:A:VAL:HG11	1:35:A:SER:H	13	0.13
(3,353)	1:31:A:VAL:HG12	1:35:A:SER:H	13	0.13
(3,353)	1:31:A:VAL:HG13	1:35:A:SER:H	13	0.13
(3,353)	1:31:A:VAL:HG11	1:35:A:SER:H	20	0.13
(3,353)	1:31:A:VAL:HG12	1:35:A:SER:H	20	0.13
(3,353)	1:31:A:VAL:HG13	1:35:A:SER:H	20	0.13
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	5	0.13
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	20	0.13
(3,123)	1:21:A:HIS:HA	1:115:A:ASP:HB2	17	0.13
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	17	0.13
(3,19)	1:11:A:SER:HA	1:13:A:TYR:HB3	20	0.13
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	5	0.13
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	13	0.13
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	19	0.13
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	15	0.13
(2,16)	1:61:A:GLN:N	1:106:A:TYR:O	19	0.13
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	8	0.13
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	17	0.13
(1,11)	2:201:A:CA:CA	2:202:A:CA:CA	5	0.13
(1,9)	2:203:A:CA:CA	1:126:A:VAL:O	8	0.13
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	3	0.13
(1,4)	2:201:A:CA:CA	1:125:A:ASP:OD2	10	0.13
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	12	0.12
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	14	0.12
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	15	0.12
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	18	0.12
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	2	0.12
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	4	0.12
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	6	0.12
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	8	0.12
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	13	0.12
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	2	0.12
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	5	0.12
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	6	0.12
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	9	0.12
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	19	0.12
(3,1810)	1:116:A:LEU:HG	1:118:A:VAL:HG21	11	0.12
(3,1810)	1:116:A:LEU:HG	1:118:A:VAL:HG22	11	0.12
(3,1810)	1:116:A:LEU:HG	1:118:A:VAL:HG23	11	0.12
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	2	0.12
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	5	0.12
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	14	0.12
(3,1652)	1:107:A:VAL:H	1:115:A:ASP:HA	17	0.12
(3,1649)	1:107:A:VAL:H	1:116:A:LEU:H	20	0.12
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	18	0.12
(3,1639)	1:107:A:VAL:H	1:114:A:THR:HB	15	0.12
(3,1606)	1:105:A:ILE:H	1:116:A:LEU:HA	3	0.12
(3,1606)	1:105:A:ILE:H	1:116:A:LEU:HA	6	0.12
(3,1561)	1:104:A:GLN:HA	1:118:A:VAL:H	12	0.12
(3,1532)	1:103:A:LEU:H	1:119:A:LEU:HB2	17	0.12
(3,1498)	1:102:A:ASP:HB2	1:120:A:THR:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	6	0.12
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	5	0.12
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	11	0.12
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	2	0.12
(3,1227)	1:77:A:LEU:HG	1:83:A:GLU:H	18	0.12
(3,1186)	1:75:A:ASN:H	1:82:A:PHE:HA	15	0.12
(3,1140)	1:74:A:VAL:HA	1:85:A:VAL:HA	6	0.12
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	3	0.12
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	3	0.12
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	3	0.12
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	3	0.12
(3,1003)	1:67:A:PRO:HD2	1:101:A:PHE:HB3	13	0.12
(3,1003)	1:67:A:PRO:HD3	1:101:A:PHE:HB3	13	0.12
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	12	0.12
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	17	0.12
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	18	0.12
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	19	0.12
(3,848)	1:62:A:ILE:HG21	1:103:A:LEU:HA	19	0.12
(3,848)	1:62:A:ILE:HG22	1:103:A:LEU:HA	19	0.12
(3,848)	1:62:A:ILE:HG23	1:103:A:LEU:HA	19	0.12
(3,844)	1:62:A:ILE:HG12	1:74:A:VAL:HA	19	0.12
(3,611)	1:46:A:VAL:HB	1:81:A:TYR:HA	19	0.12
(3,603)	1:45:A:SER:H	1:81:A:TYR:HA	1	0.12
(3,603)	1:45:A:SER:H	1:81:A:TYR:HA	3	0.12
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	19	0.12
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	1	0.12
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	7	0.12
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	1	0.12
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	13	0.12
(3,511)	1:41:A:VAL:H	1:83:A:GLU:HB3	18	0.12
(3,466)	1:39:A:THR:HB	1:86:A:THR:H	9	0.12
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	6	0.12
(3,300)	1:29:A:GLY:HA2	1:121:A:VAL:H	20	0.12
(3,224)	1:24:A:LEU:HG	1:44:A:PHE:HA	11	0.12
(3,142)	1:22:A:LEU:H	1:115:A:ASP:HB3	6	0.12
(3,121)	1:21:A:HIS:HB2	1:47:A:LYS:HB2	2	0.12
(3,121)	1:21:A:HIS:HB2	1:47:A:LYS:HB3	2	0.12
(3,121)	1:21:A:HIS:HB3	1:47:A:LYS:HB2	2	0.12
(3,121)	1:21:A:HIS:HB3	1:47:A:LYS:HB3	2	0.12
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	15	0.12
(3,34)	1:13:A:TYR:HB3	1:15:A:ASP:H	15	0.12
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	20	0.12
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	17	0.12
(1,2)	2:201:A:CA:CA	1:95:A:GLU:OE2	15	0.12
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	6	0.11
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	1	0.11
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	2	0.11
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	11	0.11
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	20	0.11
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	19	0.11
(4,10)	1:29:A:GLY:H	1:120:A:THR:O	20	0.11
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	3	0.11
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	7	0.11
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	10	0.11
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	15	0.11
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	17	0.11
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	8	0.11
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	10	0.11
(3,1789)	1:114:A:THR:H	1:115:A:ASP:HB3	2	0.11
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	8	0.11
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	13	0.11
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	19	0.11
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	4	0.11
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	6	0.11
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	7	0.11
(3,1690)	1:108:A:LYS:HA	1:113:A:VAL:H	15	0.11
(3,1671)	1:108:A:LYS:HB2	1:112:A:GLY:HA2	8	0.11
(3,1653)	1:107:A:VAL:H	1:114:A:THR:HA	20	0.11
(3,1652)	1:107:A:VAL:H	1:115:A:ASP:HA	7	0.11
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	2	0.11
(3,1648)	1:107:A:VAL:H	1:115:A:ASP:HB2	6	0.11
(3,1589)	1:105:A:ILE:HD11	1:119:A:LEU:HG	18	0.11
(3,1589)	1:105:A:ILE:HD12	1:119:A:LEU:HG	18	0.11
(3,1589)	1:105:A:ILE:HD13	1:119:A:LEU:HG	18	0.11
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	1	0.11
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	3	0.11
(3,1581)	1:105:A:ILE:HB	1:119:A:LEU:HG	9	0.11
(3,1572)	1:104:A:GLN:HG2	1:118:A:VAL:HA	11	0.11
(3,1572)	1:104:A:GLN:HG3	1:118:A:VAL:HA	11	0.11
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	5	0.11
(3,1486)	1:101:A:PHE:HB2	1:121:A:VAL:H	17	0.11
(3,1486)	1:101:A:PHE:HB2	1:121:A:VAL:H	20	0.11
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	11	0.11
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	1	0.11
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	6	0.11
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	1	0.11
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	19	0.11
(3,1430)	1:97:A:GLY:HA2	1:98:A:PRO:HA	9	0.11
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	6	0.11
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	7	0.11
(3,1237)	1:77:A:LEU:HA	1:83:A:GLU:H	17	0.11
(3,1203)	1:76:A:TRP:HA	1:77:A:LEU:HG	2	0.11
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	16	0.11
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	9	0.11
(3,1105)	1:73:A:ARG:HG3	1:85:A:VAL:HA	16	0.11
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	1	0.11
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	6	0.11
(3,1065)	1:71:A:ALA:HA	1:90:A:GLU:H	2	0.11
(3,1064)	1:71:A:ALA:HA	1:87:A:THR:H	3	0.11
(3,1058)	1:71:A:ALA:HB1	1:92:A:LEU:HG	5	0.11
(3,1058)	1:71:A:ALA:HB2	1:92:A:LEU:HG	5	0.11
(3,1058)	1:71:A:ALA:HB3	1:92:A:LEU:HG	5	0.11
(3,1036)	1:70:A:GLU:HA	1:90:A:GLU:HA	6	0.11
(3,1022)	1:68:A:LEU:HG	1:69:A:THR:H	18	0.11
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	2	0.11
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	2	0.11
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	5	0.11
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	5	0.11
(3,1008)	1:67:A:PRO:HD2	1:101:A:PHE:HB2	11	0.11
(3,1008)	1:67:A:PRO:HD3	1:101:A:PHE:HB2	11	0.11
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	15	0.11
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	5	0.11
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	9	0.11
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	15	0.11
(3,949)	1:64:A:ASN:H	1:105:A:ILE:HA	20	0.11
(3,938)	1:64:A:ASN:H	1:105:A:ILE:H	9	0.11
(3,938)	1:64:A:ASN:H	1:105:A:ILE:H	17	0.11
(3,868)	1:62:A:ILE:H	1:105:A:ILE:HA	5	0.11
(3,868)	1:62:A:ILE:H	1:105:A:ILE:HA	19	0.11
(3,814)	1:61:A:GLN:H	1:108:A:LYS:H	9	0.11
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	6	0.11
(3,789)	1:60:A:PRO:HB3	1:107:A:VAL:H	17	0.11
(3,704)	1:53:A:SER:H	1:110:A:GLU:H	16	0.11
(3,582)	1:44:A:PHE:H	1:82:A:PHE:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	7	0.11
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	8	0.11
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	15	0.11
(3,569)	1:43:A:LYS:HB2	1:83:A:GLU:H	18	0.11
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	9	0.11
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	11	0.11
(3,533)	1:42:A:HIS:HA	1:84:A:VAL:HB	18	0.11
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	10	0.11
(3,429)	1:37:A:PRO:HA	1:87:A:THR:H	15	0.11
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	15	0.11
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB2	11	0.11
(3,381)	1:32:A:ALA:H	1:35:A:SER:HB3	11	0.11
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	2	0.11
(3,355)	1:31:A:VAL:H	1:41:A:VAL:HB	3	0.11
(3,322)	1:30:A:ASN:H	1:122:A:GLN:HG2	8	0.11
(3,300)	1:29:A:GLY:HA2	1:121:A:VAL:H	2	0.11
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	7	0.11
(3,116)	1:21:A:HIS:HA	1:115:A:ASP:HB3	3	0.11
(3,116)	1:21:A:HIS:HA	1:115:A:ASP:HB3	7	0.11
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	4	0.11
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	12	0.11
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	1	0.11
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	13	0.11
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	2	0.11
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	14	0.11
(1,12)	2:201:A:CA:CA	2:203:A:CA:CA	7	0.11
(1,10)	2:203:A:CA:CA	1:127:A:ASN:OD1	11	0.11
(1,5)	2:202:A:CA:CA	1:33:A:GLU:OE1	11	0.11
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	3	0.1
(4,51)	1:107:A:VAL:O	1:115:A:ASP:H	16	0.1
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	7	0.1
(4,36)	1:73:A:ARG:H	1:85:A:VAL:O	15	0.1
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	10	0.1
(4,13)	1:38:A:GLY:H	1:86:A:THR:O	13	0.1
(4,7)	1:27:A:ALA:O	1:120:A:THR:H	9	0.1
(4,5)	1:23:A:ILE:O	1:45:A:SER:H	7	0.1
(3,1865)	1:121:A:VAL:HA	1:123:A:VAL:H	8	0.1
(3,1848)	1:119:A:LEU:HA	1:121:A:VAL:H	19	0.1
(3,1800)	1:115:A:ASP:HB3	1:117:A:GLN:HG2	17	0.1
(3,1800)	1:115:A:ASP:HB3	1:117:A:GLN:HG3	17	0.1
(3,1749)	1:111:A:VAL:H	1:112:A:GLY:HA3	1	0.1
(3,1694)	1:108:A:LYS:HG3	1:113:A:VAL:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1653)	1:107:A:VAL:H	1:114:A:THR:HA	5	0.1
(3,1639)	1:107:A:VAL:H	1:114:A:THR:HB	1	0.1
(3,1599)	1:105:A:ILE:HB	1:119:A:LEU:H	10	0.1
(3,1488)	1:101:A:PHE:HB3	1:121:A:VAL:HB	3	0.1
(3,1486)	1:101:A:PHE:HB2	1:121:A:VAL:H	1	0.1
(3,1482)	1:101:A:PHE:H	1:120:A:THR:HB	8	0.1
(3,1458)	1:100:A:ILE:H	1:122:A:GLN:HG2	8	0.1
(3,1452)	1:100:A:ILE:HB	1:102:A:ASP:HA	19	0.1
(3,1440)	1:99:A:ASN:H	1:123:A:VAL:HB	19	0.1
(3,1433)	1:99:A:ASN:HA	1:122:A:GLN:HG3	3	0.1
(3,1191)	1:75:A:ASN:HB2	1:83:A:GLU:H	14	0.1
(3,1107)	1:73:A:ARG:HB2	1:74:A:VAL:HA	4	0.1
(3,1103)	1:73:A:ARG:HB2	1:88:A:GLY:HA3	13	0.1
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	7	0.1
(3,1073)	1:72:A:PHE:H	1:85:A:VAL:H	19	0.1
(3,993)	1:66:A:ASN:HB3	1:101:A:PHE:H	10	0.1
(3,989)	1:66:A:ASN:H	1:103:A:LEU:H	19	0.1
(3,959)	1:65:A:SER:HA	1:101:A:PHE:HA	12	0.1
(3,938)	1:64:A:ASN:H	1:105:A:ILE:H	18	0.1
(3,927)	1:64:A:ASN:HB2	1:103:A:LEU:HA	8	0.1
(3,926)	1:64:A:ASN:H	1:116:A:LEU:HG	9	0.1
(3,849)	1:62:A:ILE:HB	1:73:A:ARG:HA	17	0.1
(3,822)	1:61:A:GLN:HA	1:74:A:VAL:HB	2	0.1
(3,822)	1:61:A:GLN:HA	1:74:A:VAL:HB	3	0.1
(3,822)	1:61:A:GLN:HA	1:74:A:VAL:HB	4	0.1
(3,791)	1:60:A:PRO:HB2	1:106:A:TYR:H	18	0.1
(3,697)	1:52:A:LEU:H	1:52:A:LEU:HB3	4	0.1
(3,547)	1:42:A:HIS:H	1:85:A:VAL:HA	20	0.1
(3,414)	1:34:A:ASN:H	1:126:A:VAL:HB	9	0.1
(3,120)	1:21:A:HIS:HA	1:47:A:LYS:H	3	0.1
(2,33)	1:101:A:PHE:H	1:121:A:VAL:O	16	0.1
(2,15)	1:61:A:GLN:H	1:106:A:TYR:O	19	0.1
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	11	0.1
(1,13)	2:202:A:CA:CA	2:203:A:CA:CA	16	0.1

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

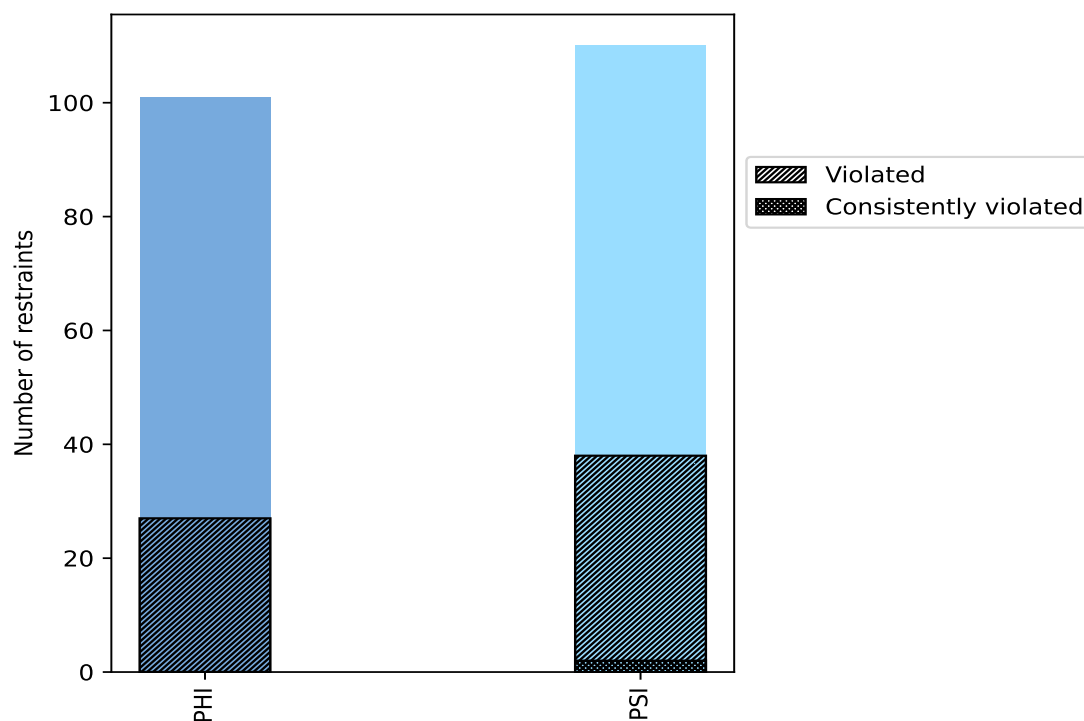
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	101	47.9	27	26.7	12.8	0	0.0	0.0
PSI	110	52.1	38	34.5	18.0	2	1.8	0.9
Total	211	100.0	65	30.8	30.8	2	0.9	0.9

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



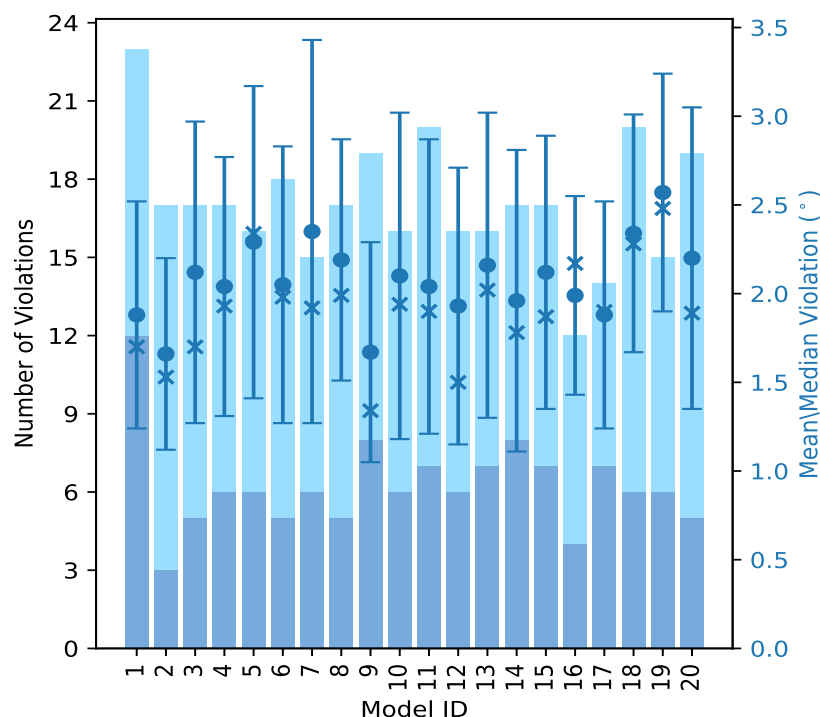
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	12	11	23	1.88	3.09	0.64	1.7
2	3	14	17	1.66	2.75	0.54	1.53
3	5	12	17	2.12	3.56	0.85	1.7
4	6	11	17	2.04	3.46	0.73	1.93
5	6	10	16	2.29	3.99	0.88	2.34
6	5	13	18	2.05	4.07	0.78	1.98
7	6	9	15	2.35	4.94	1.08	1.92
8	5	12	17	2.19	3.51	0.68	1.99
9	8	11	19	1.67	3.15	0.62	1.34
10	6	10	16	2.1	4.12	0.92	1.94
11	7	13	20	2.04	3.86	0.83	1.9
12	6	10	16	1.93	3.65	0.78	1.5
13	7	9	16	2.16	3.98	0.86	2.02
14	8	9	17	1.96	4.5	0.85	1.78
15	7	10	17	2.12	4.17	0.77	1.87
16	4	8	12	1.99	2.73	0.56	2.17
17	7	7	14	1.88	3.19	0.64	1.9
18	6	14	20	2.34	3.67	0.67	2.28
19	6	9	15	2.57	4.1	0.67	2.48
20	5	14	19	2.2	4.11	0.85	1.89

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
7	13	20	1	5.0
4	6	10	2	10.0
4	2	6	3	15.0
4	1	5	4	20.0
1	2	3	5	25.0
1	2	3	6	30.0
0	1	1	7	35.0
0	1	1	8	40.0
1	1	2	9	45.0
1	3	4	10	50.0
1	0	1	11	55.0

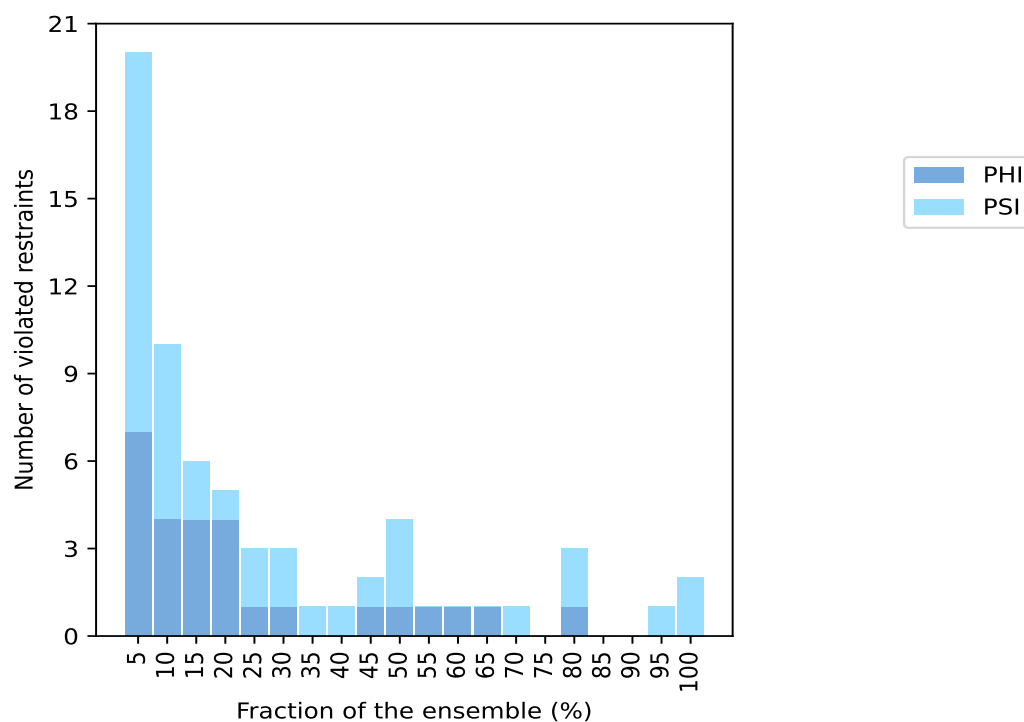
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	0	1	12	60.0
1	0	1	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
1	2	3	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
0	2	2	20	100.0

¹ Number of models with violations

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

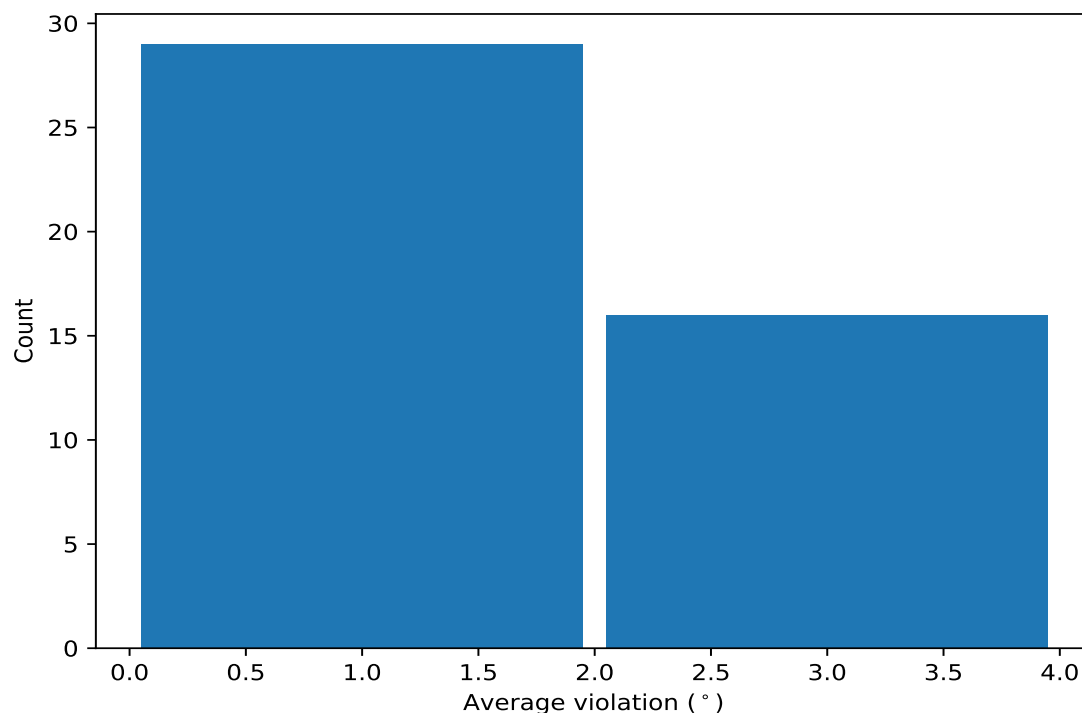


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	20	3.05	0.63	3.1
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	20	2.3	0.46	2.34
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	19	2.58	0.51	2.59
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	16	2.51	0.64	2.46
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	16	2.38	0.49	2.24
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	16	1.66	0.32	1.58
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	14	1.87	0.7	1.6
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	13	1.77	0.57	1.55
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	12	2.79	0.77	2.79
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	11	2.44	0.94	2.25
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	10	3.69	0.54	3.74
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	10	1.74	0.7	1.61
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	10	1.61	0.45	1.51
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	10	1.36	0.3	1.27
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	9	2.13	0.52	2.14
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	9	1.41	0.26	1.3
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	8	2.71	0.49	2.7
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	7	1.36	0.25	1.34
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	6	2.28	0.92	2.34
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	6	2.17	0.55	2.27

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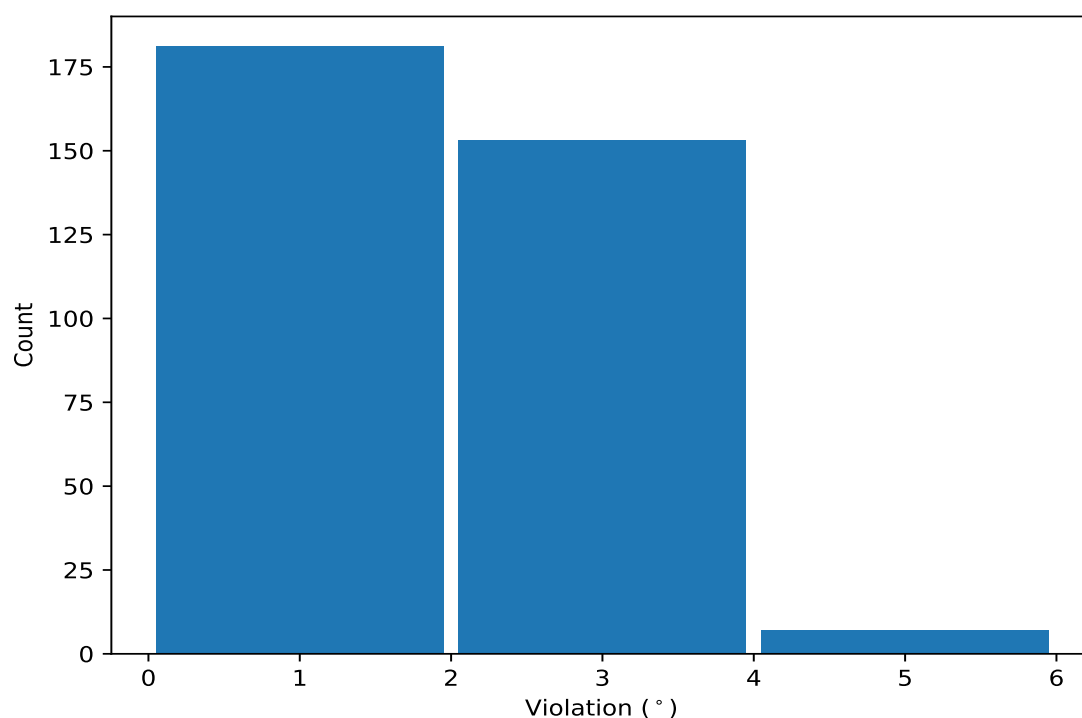
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	6	1.48	0.43	1.36
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	5	2.06	0.78	2.63
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	5	1.33	0.15	1.27
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	5	1.24	0.12	1.2
(1,150)	1:95:A:GLU:C	1:96:A:THR:N	1:96:A:THR:CA	1:96:A:THR:C	4	2.26	0.55	1.96
(1,17)	1:20:A:LEU:C	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	4	1.97	0.65	1.83
(1,96)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:PRO:N	4	1.53	0.39	1.54
(1,140)	1:90:A:GLU:C	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	4	1.34	0.21	1.4
(1,75)	1:54:A:PRO:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	4	1.32	0.11	1.36
(1,35)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:VAL:N	3	2.12	0.45	1.81
(1,145)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:PHE:N	3	2.1	0.49	2.11
(1,54)	1:43:A:LYS:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	3	1.84	0.87	1.37
(1,100)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	3	1.83	0.89	1.22
(1,48)	1:40:A:SER:C	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	3	1.58	0.75	1.1
(1,15)	1:19:A:LYS:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	3	1.52	0.45	1.39
(1,98)	1:67:A:PRO:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	2	1.89	0.07	1.89
(1,182)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	2	1.8	0.48	1.8
(1,99)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	2	1.71	0.01	1.71
(1,69)	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1:52:A:LEU:N	2	1.63	0.37	1.63
(1,41)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:SER:N	2	1.46	0.16	1.46
(1,95)	1:65:A:SER:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	2	1.46	0.38	1.46
(1,106)	1:72:A:PHE:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	2	1.44	0.32	1.44
(1,146)	1:93:A:ASP:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	2	1.36	0.2	1.36
(1,47)	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	1:41:A:VAL:N	2	1.23	0.13	1.23
(1,31)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:GLY:N	2	1.04	0.03	1.04

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	7	4.94
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	14	4.5
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	15	4.17
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	10	4.12
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	20	4.11
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	19	4.1
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	6	4.07
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	5	3.99
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	13	3.98
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	11	3.86
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	20	3.76
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	5	3.74
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	7	3.73
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	13	3.73
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	18	3.67
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	12	3.65
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	7	3.58
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	3	3.56
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	8	3.51
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	19	3.5
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	3	3.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	18	3.48
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	11	3.47
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	8	3.47
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	4	3.46
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	15	3.42
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	3	3.37
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	3	3.27
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	14	3.26
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	4	3.25
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	18	3.23
(1,150)	1:95:A:GLU:C	1:96:A:THR:N	1:96:A:THR:CA	1:96:A:THR:C	18	3.22
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	7	3.22
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	13	3.22
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	10	3.2
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	19	3.19
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	17	3.19
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	20	3.19
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	9	3.15
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	10	3.12
(1,100)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1	3.09
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	5	3.08
(1,54)	1:43:A:LYS:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	1	3.06
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	7	3.02
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	4	3.01
(1,17)	1:20:A:LEU:C	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	19	3.0
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	10	2.98
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	12	2.98
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	5	2.96
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	5	2.94
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	11	2.92
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	8	2.91
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	4	2.89
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	12	2.88
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	20	2.88
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	20	2.87
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1	2.86
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	6	2.85
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	8	2.84
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	6	2.83
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	11	2.8
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	20	2.8
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	1	2.79
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	19	2.78
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	2	2.75
(1,35)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:VAL:N	18	2.75
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	6	2.75
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	20	2.74
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	15	2.74
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	6	2.74
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	19	2.74
(1,176)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:GLY:N	16	2.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	10	2.73
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	13	2.72
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	12	2.71
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	8	2.71
(1,145)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:PHE:N	2	2.7
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	16	2.69
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	1	2.69
(1,204)	1:125:A:ASP:N	1:125:A:ASP:CA	1:125:A:ASP:C	1:126:A:VAL:N	17	2.68
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	3	2.67
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	11	2.65
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1	2.64
(1,48)	1:40:A:SER:C	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	11	2.64
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	9	2.63
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	15	2.63
(1,147)	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	1:95:A:GLU:N	12	2.61
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	17	2.6
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	11	2.59
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	11	2.59
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	19	2.59
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	16	2.56
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	10	2.55
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	5	2.53
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	14	2.53
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	18	2.52
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	6	2.5
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	14	2.5
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	3	2.49
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	19	2.48
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	16	2.47
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	15	2.46
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	9	2.46
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	5	2.46
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	9	2.45
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	19	2.45
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	15	2.44
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	8	2.41
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	2	2.41
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	5	2.41
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	13	2.41
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	18	2.41
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	3	2.37
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	18	2.37
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	18	2.36
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	7	2.36
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	6	2.35
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	4	2.34
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	10	2.34
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	17	2.33
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	13	2.31
(1,149)	1:95:A:GLU:N	1:95:A:GLU:CA	1:95:A:GLU:C	1:96:A:THR:N	18	2.29
(1,182)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	18	2.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,208)	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	1:128:A:GLU:N	5	2.26
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	7	2.26
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	18	2.26
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	8	2.25
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	8	2.25
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	5	2.25
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	10	2.23
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	19	2.23
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	16	2.22
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	19	2.21
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	9	2.19
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	16	2.19
(1,16)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:HIS:N	20	2.19
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	6	2.17
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	16	2.15
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	15	2.14
(1,15)	1:19:A:LYS:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	14	2.13
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	12	2.12
(1,145)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:PHE:N	4	2.11
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	6	2.11
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	4	2.1
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	2	2.1
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	13	2.09
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	12	2.08
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	19	2.08
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	18	2.08
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	4	2.08
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	18	2.08
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	11	2.08
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	18	2.06
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	18	2.05
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	13	2.04
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	17	2.04
(1,119)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:THR:N	1	2.0
(1,96)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:PRO:N	3	2.0
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	13	2.0
(1,69)	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1:52:A:LEU:N	18	2.0
(1,150)	1:95:A:GLU:C	1:96:A:THR:N	1:96:A:THR:CA	1:96:A:THR:C	19	1.99
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	8	1.99
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	17	1.98
(1,105)	1:72:A:PHE:N	1:72:A:PHE:CA	1:72:A:PHE:C	1:73:A:ARG:N	8	1.97
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	14	1.97
(1,98)	1:67:A:PRO:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	14	1.96
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	20	1.96
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	13	1.95
(1,148)	1:94:A:PHE:C	1:95:A:GLU:N	1:95:A:GLU:CA	1:95:A:GLU:C	15	1.94
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	8	1.94
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	13	1.94
(1,150)	1:95:A:GLU:C	1:96:A:THR:N	1:96:A:THR:CA	1:96:A:THR:C	1	1.93
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	4	1.93
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	11	1.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	1	1.92
(1,150)	1:95:A:GLU:C	1:96:A:THR:N	1:96:A:THR:CA	1:96:A:THR:C	4	1.92
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	7	1.92
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	17	1.91
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	20	1.89
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	17	1.88
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	2	1.88
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	15	1.87
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	9	1.87
(1,17)	1:20:A:LEU:C	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	9	1.87
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	20	1.86
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	6	1.86
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	11	1.86
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	19	1.86
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	15	1.85
(1,95)	1:65:A:SER:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	14	1.84
(1,4)	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	1:13:A:TYR:N	6	1.83
(1,98)	1:67:A:PRO:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1	1.82
(1,35)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:VAL:N	2	1.81
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	17	1.8
(1,96)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:PRO:N	8	1.8
(1,35)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:VAL:N	15	1.8
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	1	1.8
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	2	1.8
(1,17)	1:20:A:LEU:C	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	14	1.78
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	8	1.77
(1,106)	1:72:A:PHE:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	4	1.76
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	14	1.74
(1,34)	1:29:A:GLY:C	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	20	1.73
(1,99)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	14	1.72
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	4	1.72
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	5	1.71
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	7	1.7
(1,99)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:THR:N	1	1.7
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	3	1.7
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	7	1.69
(1,28)	1:26:A:PRO:C	1:27:A:ALA:N	1:27:A:ALA:CA	1:27:A:ALA:C	3	1.68
(1,8)	1:16:A:ASP:N	1:16:A:ASP:CA	1:16:A:ASP:C	1:17:A:ASP:N	3	1.67
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	7	1.66
(1,79)	1:57:A:PRO:N	1:57:A:PRO:CA	1:57:A:PRO:C	1:58:A:GLY:N	10	1.64
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	1	1.64
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	9	1.63
(1,41)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:SER:N	10	1.63
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	16	1.62
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	3	1.6
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	9	1.6
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	3	1.59
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	1	1.59
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	4	1.56
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	15	1.56
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	15	1.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	2	1.56
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	11	1.55
(1,146)	1:93:A:ASP:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	15	1.55
(1,115)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:SER:N	16	1.55
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	7	1.53
(1,140)	1:90:A:GLU:C	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	2	1.53
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	15	1.53
(1,140)	1:90:A:GLU:C	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	12	1.52
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	18	1.52
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	1	1.52
(1,145)	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1:94:A:PHE:N	12	1.49
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	13	1.49
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	8	1.48
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	20	1.48
(1,7)	1:15:A:ASP:C	1:16:A:ASP:N	1:16:A:ASP:CA	1:16:A:ASP:C	12	1.48
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	1	1.47
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	5	1.46
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	14	1.46
(1,57)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:VAL:N	20	1.46
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	20	1.45
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	20	1.44
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	6	1.44
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	1	1.42
(1,75)	1:54:A:PRO:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	5	1.42
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	6	1.41
(1,207)	1:126:A:VAL:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	8	1.4
(1,75)	1:54:A:PRO:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1	1.4
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	20	1.39
(1,15)	1:19:A:LYS:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	2	1.39
(1,54)	1:43:A:LYS:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	3	1.37
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	12	1.36
(1,47)	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	1:41:A:VAL:N	2	1.36
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	6	1.36
(1,102)	1:69:A:THR:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	14	1.35
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	13	1.34
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	10	1.34
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	9	1.34
(1,60)	1:46:A:VAL:C	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	13	1.34
(1,182)	1:114:A:THR:N	1:114:A:THR:CA	1:114:A:THR:C	1:115:A:ASP:N	19	1.32
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	8	1.31
(1,75)	1:54:A:PRO:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	16	1.31
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	10	1.31
(1,11)	1:17:A:ASP:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	11	1.31
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	9	1.3
(1,83)	1:59:A:PHE:N	1:59:A:PHE:CA	1:59:A:PHE:C	1:60:A:PRO:N	20	1.3
(1,44)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:PRO:N	17	1.3
(1,41)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:SER:N	9	1.3
(1,10)	1:17:A:ASP:N	1:17:A:ASP:CA	1:17:A:ASP:C	1:18:A:ASP:N	2	1.3
(1,140)	1:90:A:GLU:C	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1	1.29
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	11	1.29
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	9	1.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:89:A:MET:N	1:89:A:MET:CA	1:89:A:MET:C	1:90:A:GLU:N	7	1.28
(1,96)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:PRO:N	11	1.28
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	5	1.27
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	12	1.27
(1,69)	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1:52:A:LEU:N	2	1.26
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	11	1.25
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	6	1.24
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	8	1.24
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	11	1.24
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	1	1.24
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	12	1.24
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	15	1.23
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	6	1.23
(1,100)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	9	1.22
(1,17)	1:20:A:LEU:C	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	16	1.22
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	20	1.22
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	12	1.21
(1,85)	1:60:A:PRO:C	1:61:A:GLN:N	1:61:A:GLN:CA	1:61:A:GLN:C	17	1.21
(1,24)	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	1:25:A:LEU:N	7	1.21
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	10	1.2
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	6	1.2
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	12	1.2
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	1	1.2
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	11	1.19
(1,143)	1:92:A:LEU:N	1:92:A:LEU:CA	1:92:A:LEU:C	1:93:A:ASP:N	11	1.19
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	14	1.19
(1,100)	1:68:A:LEU:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	14	1.19
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	16	1.18
(1,90)	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	1:64:A:ASN:N	17	1.18
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	15	1.18
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	1	1.17
(1,146)	1:93:A:ASP:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	4	1.16
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:LEU:N	4	1.15
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	4	1.15
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	14	1.15
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	2	1.14
(1,80)	1:57:A:PRO:C	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	17	1.13
(1,75)	1:54:A:PRO:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	2	1.13
(1,155)	1:100:A:ILE:C	1:101:A:PHE:N	1:101:A:PHE:CA	1:101:A:PHE:C	18	1.12
(1,131)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:THR:N	9	1.12
(1,106)	1:72:A:PHE:C	1:73:A:ARG:N	1:73:A:ARG:CA	1:73:A:ARG:C	12	1.11
(1,87)	1:61:A:GLN:C	1:62:A:ILE:N	1:62:A:ILE:CA	1:62:A:ILE:C	5	1.1
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	3	1.1
(1,48)	1:40:A:SER:C	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	14	1.1
(1,47)	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	1:41:A:VAL:N	10	1.1
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	7	1.1
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	9	1.09
(1,138)	1:89:A:MET:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	5	1.08
(1,95)	1:65:A:SER:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	10	1.08
(1,54)	1:43:A:LYS:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	9	1.08
(1,117)	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1:79:A:GLY:N	18	1.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:GLY:N	11	1.07
(1,12)	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	1:19:A:LYS:N	3	1.07
(1,103)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:ALA:N	2	1.06
(1,40)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	9	1.05
(1,135)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:GLY:N	9	1.04
(1,96)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:PRO:N	2	1.04
(1,15)	1:19:A:LYS:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	13	1.04
(1,184)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:LEU:N	10	1.02
(1,140)	1:90:A:GLU:C	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	17	1.02
(1,31)	1:28:A:THR:N	1:28:A:THR:CA	1:28:A:THR:C	1:29:A:GLY:N	3	1.02
(1,81)	1:58:A:GLY:N	1:58:A:GLY:CA	1:58:A:GLY:C	1:59:A:PHE:N	4	1.01
(1,48)	1:40:A:SER:C	1:41:A:VAL:N	1:41:A:VAL:CA	1:41:A:VAL:C	6	1.01
(1,18)	1:21:A:HIS:N	1:21:A:HIS:CA	1:21:A:HIS:C	1:22:A:LEU:N	13	1.01
(1,116)	1:77:A:LEU:C	1:78:A:SER:N	1:78:A:SER:CA	1:78:A:SER:C	1	1.0