wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2JR2
Title	:	Solution NMR structure of homodimer CPS_2611 from Colwellia psychrerythraea. Northeast Structural Genomics Consortium target CsR4.
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Deposited on	:	2007-06-19

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

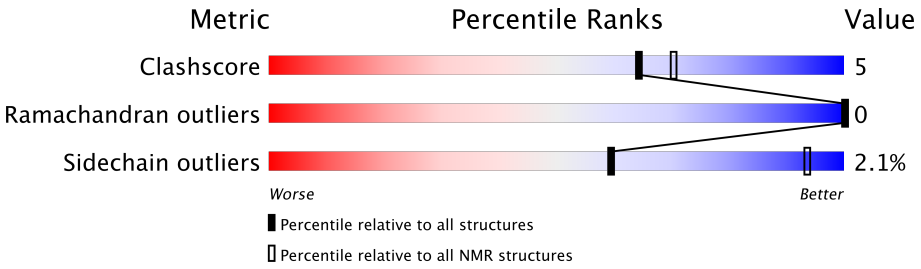
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analalysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.6.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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

Mol	Chain	Length	Quality of chain
1	A	76	78% · 18%
1	B	76	74% 7% 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:69, B:8-B:68 (123)	0.35	1

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2460 atoms, of which 1254 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UPF0352 protein CPS_2611.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1230	381	627	107	112	3	
1	B	76	Total	C	H	N	O	S	0
			1230	381	627	107	112	3	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	-	CLONING ARTIFACT	UNP Q481E4
A	70	GLU	-	CLONING ARTIFACT	UNP Q481E4
A	71	HIS	-	CLONING ARTIFACT	UNP Q481E4
A	72	HIS	-	CLONING ARTIFACT	UNP Q481E4
A	73	HIS	-	CLONING ARTIFACT	UNP Q481E4
A	74	HIS	-	CLONING ARTIFACT	UNP Q481E4
A	75	HIS	-	CLONING ARTIFACT	UNP Q481E4
A	76	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	69	LEU	-	CLONING ARTIFACT	UNP Q481E4
B	70	GLU	-	CLONING ARTIFACT	UNP Q481E4
B	71	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	72	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	73	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	74	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	75	HIS	-	CLONING ARTIFACT	UNP Q481E4
B	76	HIS	-	CLONING ARTIFACT	UNP Q481E4

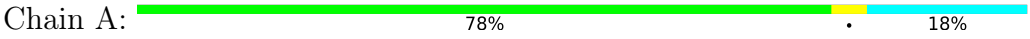
4 Residue-property plots

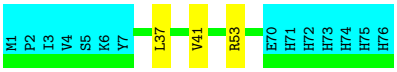
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: UPF0352 protein CPS_2611

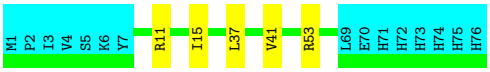
Chain A:





• Molecule 1: UPF0352 protein CPS_2611

Chain B:

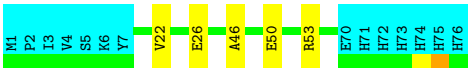


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: UPF0352 protein CPS_2611

Chain A:



• Molecule 1: UPF0352 protein CPS_2611

Chain B:

5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.15.0
CNS	refinement	1.1

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)	2jr2_nmr.cif
Number of chemical shift lists	1
Total number of shifts	1929
Number of shifts mapped to atoms	1183
Number of unparsed shifts	298
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	448
Assignment completeness (well-defined parts)	66%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	476	508	508	5±2
1	B	468	497	497	5±2
All	All	18880	20100	20100	180

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

5 of 76 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:VAL:HA	1:B:25:LYS:HE2	0.84	1.45	3	1
1:A:61:THR:HB	1:B:61:THR:HB	0.80	1.54	3	6
1:B:66:GLN:HA	1:B:66:GLN:HE21	0.74	1.42	6	1
1:A:30:PRO:HB3	1:B:48:VAL:HG22	0.67	1.66	10	1
1:A:48:VAL:O	1:A:53:ARG:HD3	0.61	1.96	18	2

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	62/76 (82%)	61±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
1	B	61/76 (80%)	60±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	2460/3040 (81%)	2432 (99%)	28 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	56/70 (80%)	55±1 (98±1%)	1±1 (2±1%)	59	93
1	B	55/70 (79%)	54±1 (98±2%)	1±1 (2±2%)	59	93
All	All	2220/2800 (79%)	2174 (98%)	46 (2%)	59	93

5 of 20 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	18	ASP	5
1	A	52	LYS	5
1	B	52	LYS	5
1	A	29	THR	4
1	B	29	THR	4

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 carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: 2jr2_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_2jr2.mr*

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	1929
Number of shifts mapped to atoms	1183
Number of unparsed shifts	298
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	448
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 298) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
5	A	2	PRO	HD%	3.370	0.020	1
17	A	3	ILE	HD1%	0.830	0.020	1
18	A	3	ILE	HD1%	0.830	0.020	1
22	A	3	ILE	HG2%	0.870	0.020	1
23	A	3	ILE	HG2%	0.870	0.020	1

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

- No matching atoms found in structure. First 5 (of 448) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	11	ARG	HB%	1.95	0.02	1
B	44	ILE	HG1x	1.01	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	30	PRO	HGy	2.12	0.02	2
B	43	ASN	HBy	2.81	0.02	2
A	16	ILE	HG1y	1.88	0.02	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	-0.40 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	146	0.40 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	142	-0.29 ± 0.12	None needed (< 0.5 ppm)
^{15}N	142	0.21 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 992 atoms were assigned a chemical shift out of a possible 1498. 35 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	601/607 (99%)	240/242 (99%)	242/246 (98%)	119/119 (100%)
Sidechain	383/873 (44%)	57/499 (11%)	308/338 (91%)	18/36 (50%)
Aromatic	8/18 (44%)	4/10 (40%)	4/8 (50%)	0/0 (—%)
Overall	992/1498 (66%)	301/751 (40%)	554/592 (94%)	137/155 (88%)

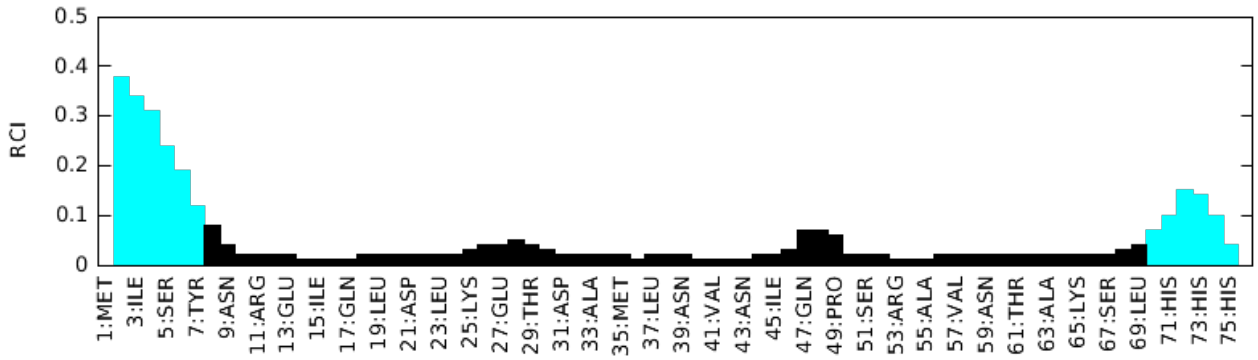
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

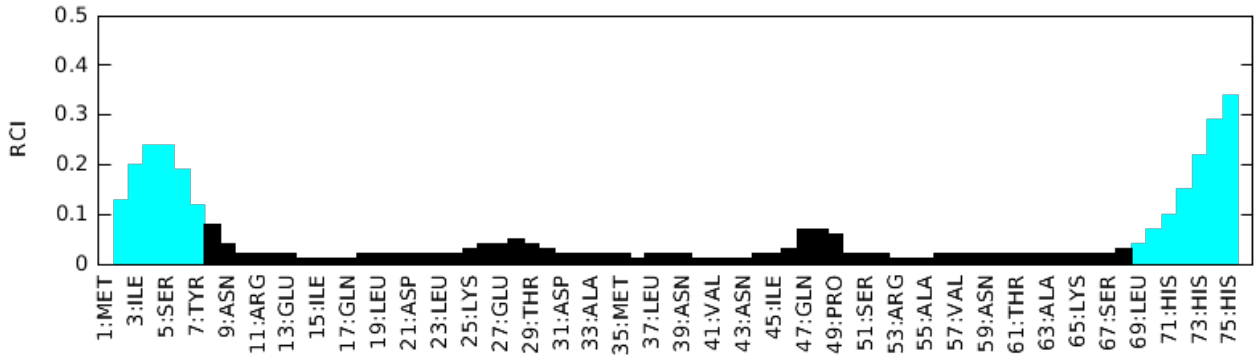
7.1.5 Random Coil Index (RCI) plots (i)

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 Distance restraints analysis

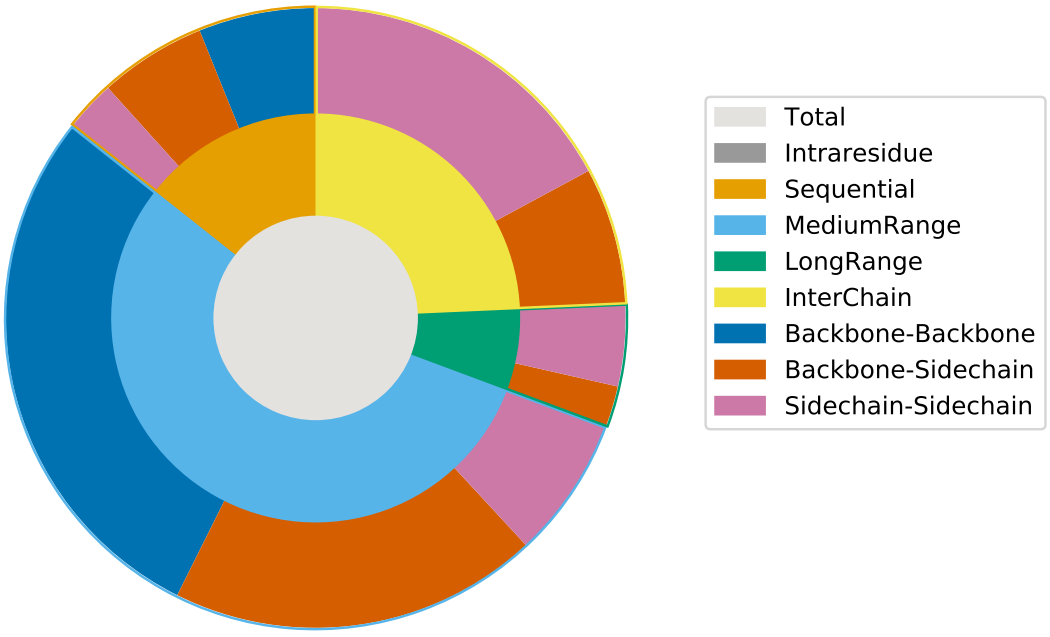
8.1 Distance restraints summary

Restraints are counted in different categories based on the atoms involved in each restraint.

Restraints type	B-B[1](H[4])	B-S[2](H[4])	S-S[3](H[4])	Total		
				Total(H[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0)	0(0)	0(0)	0(0)	0.0	0.0
Sequential (|i-j|=1)	92(0)	84(0)	40(0)	216(0)	1.6	14.3
Medium range (|i-j|>1 and |i-j|<5)	426(124)	290(0)	112(0)	828(124)	6.1	55.0
Long range (|i-j|≥5)	0(0)	32(0)	64(0)	96(0)	0.7	6.4
Inter chain	0(0)	108(0)	258(0)	366(0)	2.7	24.3
Total	518(124)	514(0)	474(0)	1506(124)	11.1	100.0

[1]number of backbone to backbone restraints, [2]number of backbone to sidechain restraints, [3]number of sidechain to sidechain restraints, [4]number of hydrogen bonds in that category, [5]number of restraints per residue, [6]percentage of restraints in that category. There are 0 unmapped restraints

8.1.1 Pie chart : Distance restraints summary



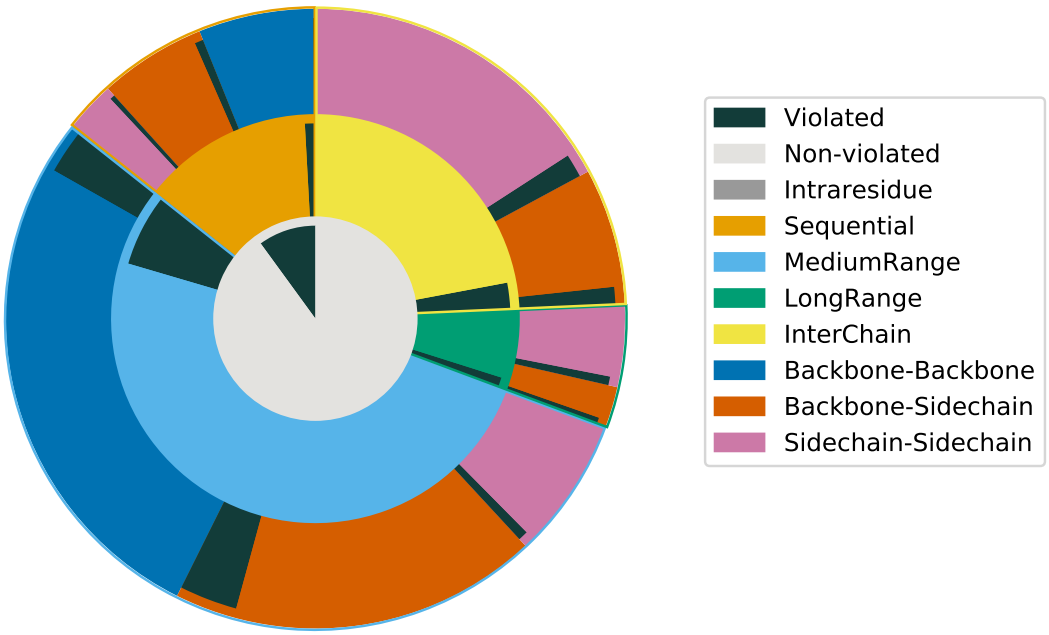
8.2 Distance violations summary

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

Restraints type	B-B[1](%[4])	B-S[2](%[4])	S-S[3](%[4])	Total		
				Total(%[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Sequential (|i-j|=1)	2(2.2)	7(8.3)	4(10.0)	13(6.0)	0.1	8.6
Medium range (|i-j|>1 and |i-j|<5)	37(8.7)	47(16.2)	8(7.1)	92(11.1)	0.7	60.9
Long range (|i-j|≥5)	0(0.0)	5(15.6)	7(10.9)	12(12.5)	0.1	7.9
Inter chain	0(0.0)	15(13.9)	19(7.4)	34(9.3)	0.3	22.5
Total	39(7.5)	74(14.4)	38(8.0)	151(10.0)	1.1	100.0

[1]number of backbone to backbone restraints, [2]number of backbone to sidechain restraints,[3]number of sidechain to sidechain restraints, [4]percentage of violations with respect to total restrains in that category, [5]number of restraints per residue, [6]percentage of violation with respect to total violations.

8.2.1 Pie-chart : Distance violations summary



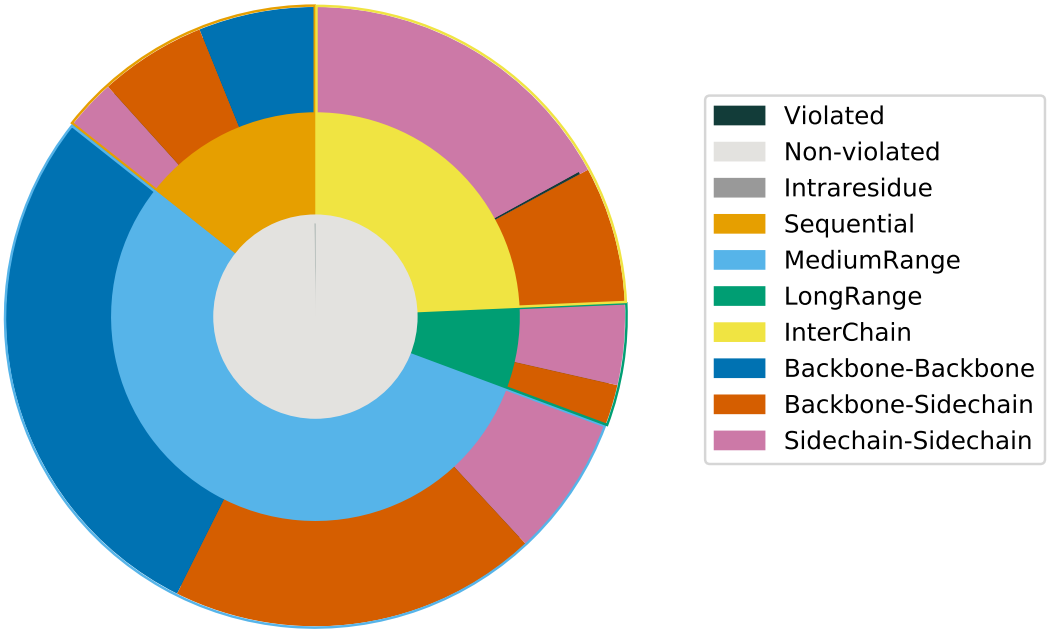
8.3 Consistent distance violations summary

The following table provides the summary of consistently violated restraints. Restraints that are violated in all models are counted as consistently violated.

Restraints type	B-B[1](%[4])	B-S[2](%[4])	S-S[3](%[4])	Total		
				Total(%[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Sequential (|i-j|=1)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Medium range (|i-j|>1 and |i-j|<5)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Long range (|i-j|≥5)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Inter chain	0(0.0)	0(0.0)	2(0.8)	2(0.5)	0.0	100.0
Total	0(0.0)	0(0.0)	2(0.4)	2(0.1)	0.0	100.0

[1]number of backbone to backbone restraints, [2]number of backbone to sidechain restraints,[3]number of sidechain to sidechain restraints, [4]percentage of violations with respect to total restrains in that category,[5]number of restraints per residue,[6]percentage of violation with respect to total violations

8.3.1 Pie-chart : Consistent distance violations



8.4 Residual distance violations

Violation are counted in different bin sizes and listed below

Range (Å)	Avg. No. of violated restraints per model	Max violation (Å)
0-0.2	19.9	0.03
0.2-0.5	None	None
0.5-1.0	None	None
1.0-2.0	None	None
2.0-5.0	None	None
5.0<	None	None

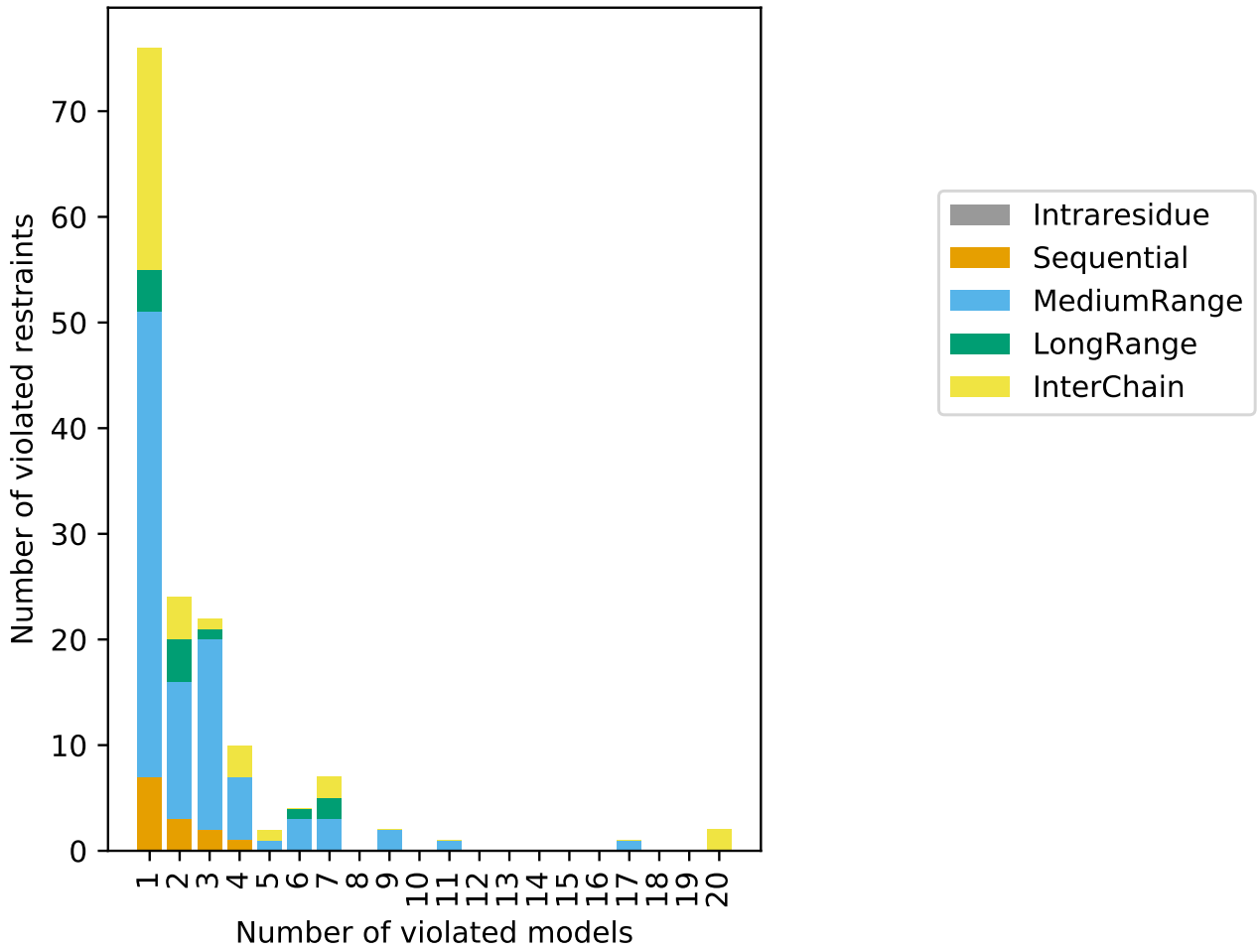
8.5 Distance violations in ensemble

The restraints are grouped based on the number of violated models and listed here.

No. of violated restraints						No. of violated models
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	
0	7	44	4	21	76	1
0	3	13	4	4	24	2
0	2	18	1	1	22	3
0	1	6	0	3	10	4
0	0	1	0	1	2	5
0	0	3	1	0	4	6
0	0	3	2	2	7	7
0	0	0	0	0	0	8
0	0	2	0	0	2	9
0	0	0	0	0	0	10
0	0	1	0	0	1	11
0	0	0	0	0	0	12
0	0	0	0	0	0	13
0	0	0	0	0	0	14
0	0	0	0	0	0	15
0	0	0	0	0	0	16
0	0	1	0	0	1	17
0	0	0	0	0	0	18
0	0	0	0	0	0	19
0	0	0	0	2	2	20

[1]intraresidue restraints, [2]sequential restraints, [3]medium range restraints, [4]long range restraints, [5]inter chain restraints

8.5.1 Bar graph : No. of models vs No. of violations



0 intraresidue restraints, 203 sequential restraints, 736 medium range restraints,84 long range restraints and 332 inter chain restraints are not violated. In total, 1355 restraints are not violated in any of the models

8.6 Violations in each model

The following table lists the violation count in each model in the ensemble

Model ID	No. of violations						Mean (Å)	Max (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total		
1	0	3	10	1	4	18	0.01	0.02
2	0	0	10	3	5	18	0.01	0.02
3	0	0	14	2	4	20	0.01	0.02
4	0	2	11	2	6	21	0.01	0.02
5	0	1	10	0	6	17	0.01	0.02

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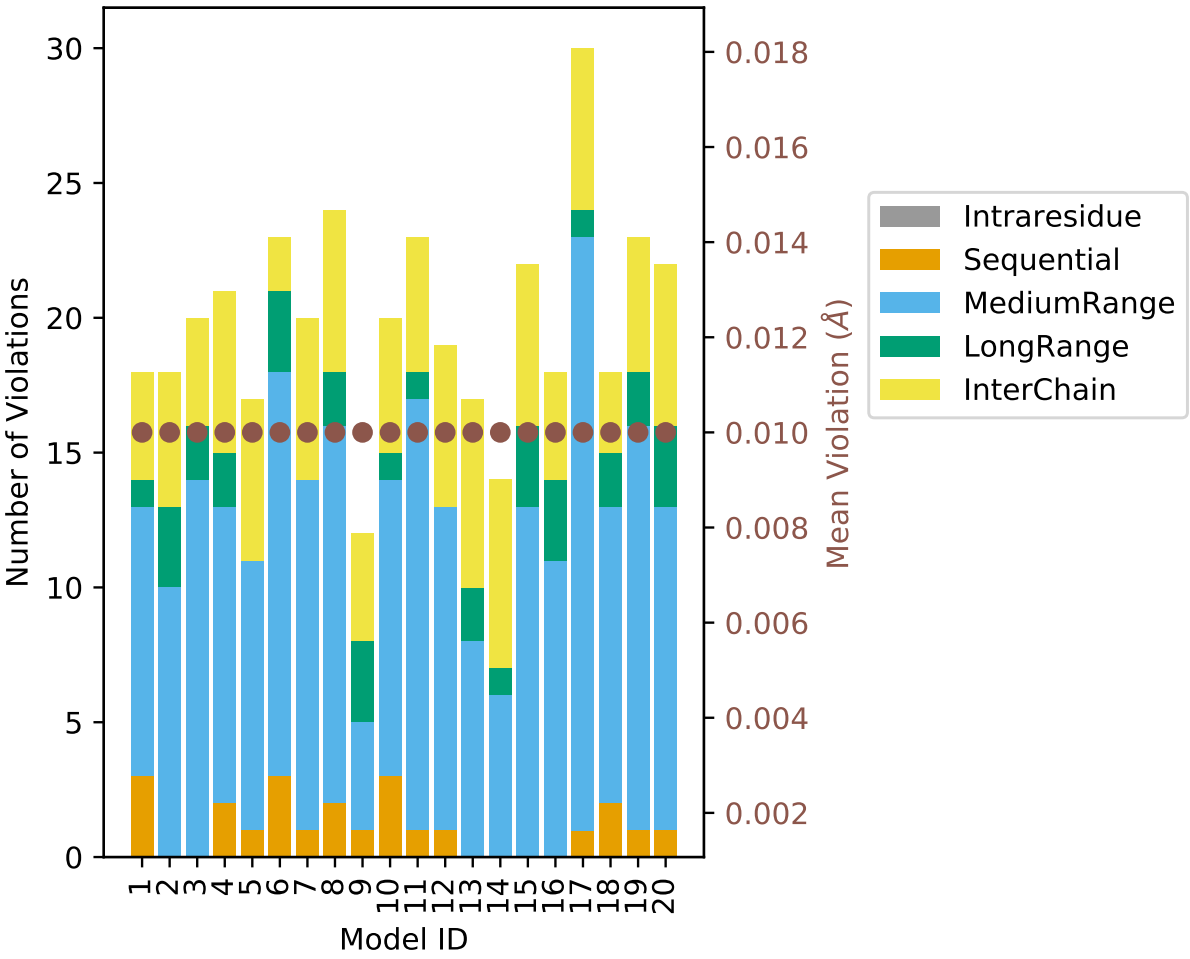
Model ID	No. of violations						Mean (Å)	Max (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total		
6	0	3	15	3	2	23	0.01	0.03
7	0	1	13	0	6	20	0.01	0.01
8	0	2	14	2	6	24	0.01	0.02
9	0	1	4	3	4	12	0.01	0.02
10	0	3	11	1	5	20	0.01	0.02
11	0	1	16	1	5	23	0.01	0.02
12	0	1	12	0	6	19	0.01	0.02
13	0	0	8	2	7	17	0.01	0.02
14	0	0	6	1	7	14	0.01	0.02
15	0	0	13	3	6	22	0.01	0.02
16	0	0	11	3	4	18	0.01	0.02
17	0	1	22	1	6	30	0.01	0.02
18	0	2	11	2	3	18	0.01	0.02
19	0	1	15	2	5	23	0.01	0.03
20	0	1	12	3	6	22	0.01	0.02

[1]intraresidue restraints, [2]iequential restraints, [3]iedium range restraints, [4]long range restraints, [5]inter chain restraints

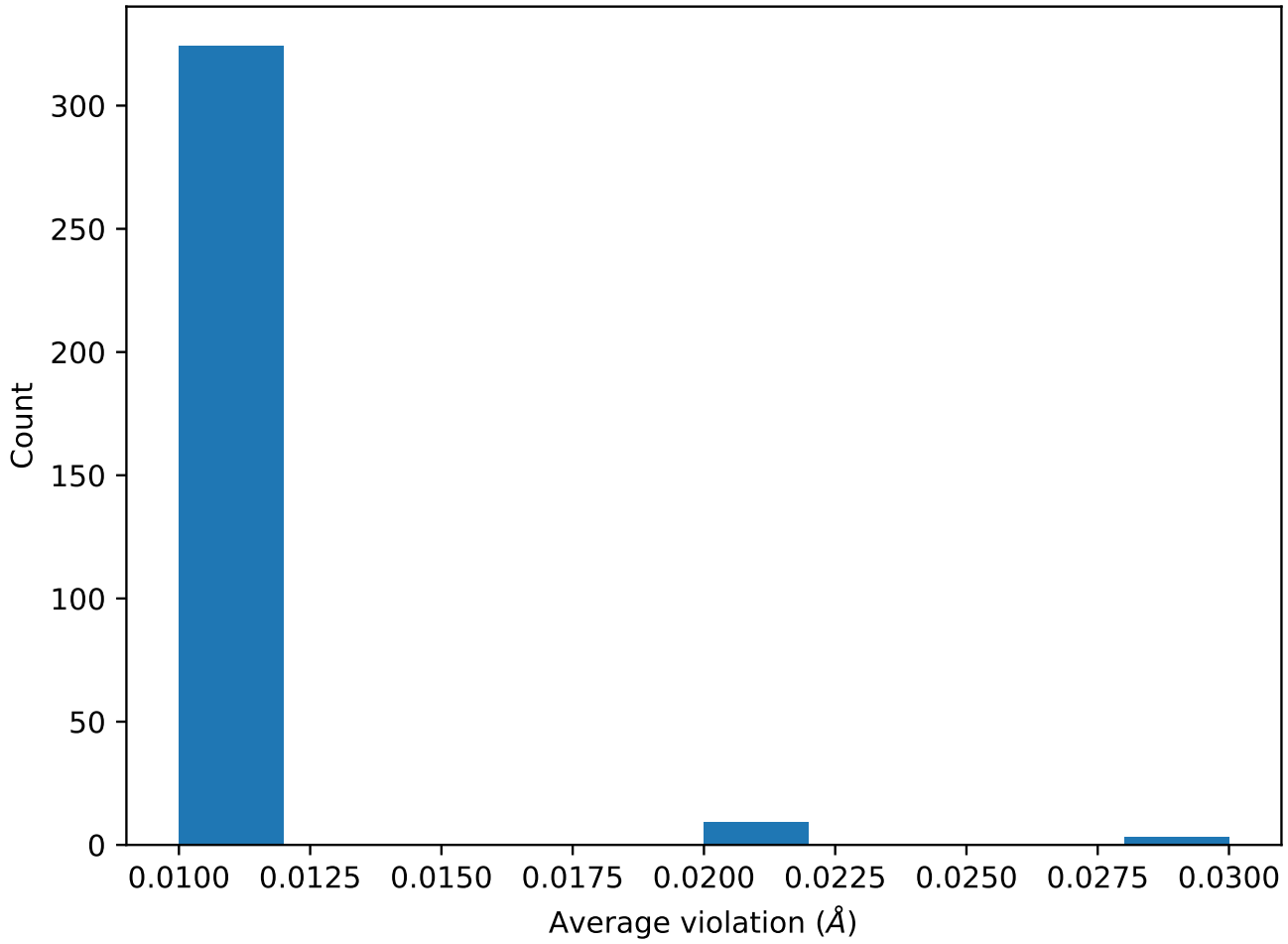
8.6.1 Bar graph : Violations in each model



8.7 Most violated distance restraints

8.7.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of average violations of each restraint.



8.7.2 Table: Most violated distance restraints

The following tale lists the average violation of each restraint sorted by number of violated models

Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	20	0.01	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	20	0.01	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	20	0.01	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	20	0.01	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	20	0.01	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	20	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	20	0.01	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	20	0.01	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	20	0.01	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	20	0.01	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	20	0.01	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	20	0.01	0.02
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	17	0.01	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	17	0.01	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	11	0.02	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	11	0.02	0.02
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	9	0.01	0.02
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	9	0.01	0.02
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	9	0.01	0.02
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	9	0.01	0.02
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	7	0.01	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	7	0.01	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	7	0.01	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	7	0.01	0.02
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	7	0.01	0.02
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	7	0.01	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	7	0.01	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	7	0.01	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	7	0.01	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	7	0.01	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	7	0.01	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	7	0.01	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	7	0.01	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	7	0.01	0.01
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	6	0.01	0.03
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	6	0.01	0.03
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	6	0.01	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	6	0.01	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	6	0.01	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	6	0.01	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	6	0.01	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	6	0.01	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	6	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	6	0.01	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	6	0.01	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	6	0.01	0.01
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	5	0.01	0.02
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	5	0.01	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	5	0.01	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	5	0.01	0.01
(1,998)	1:A:70:GLU:HA	1:A:71:HIS:H	4	0.01	0.02
(1,90)	1:B:25:LYS:N	1:B:21:ASP:O	4	0.01	0.01
(1,646)	1:A:26:GLU:HG2	1:A:28:VAL:H	4	0.01	0.01
(1,646)	1:A:26:GLU:HG3	1:A:28:VAL:H	4	0.01	0.01
(1,57)	1:A:66:GLN:N	1:A:62:LYS:O	4	0.01	0.02
(1,55)	1:A:65:LYS:N	1:A:61:THR:O	4	0.01	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG2	4	0.01	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG3	4	0.01	0.01
(1,449)	1:B:41:VAL:HG21	1:A:64:LEU:HG	4	0.01	0.01
(1,449)	1:B:41:VAL:HG22	1:A:64:LEU:HG	4	0.01	0.01
(1,449)	1:B:41:VAL:HG23	1:A:64:LEU:HG	4	0.01	0.01
(1,41)	1:A:58:ASP:N	1:A:54:VAL:O	4	0.01	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG21	4	0.01	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG22	4	0.01	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG23	4	0.01	0.01
(1,266)	1:A:41:VAL:HG21	1:B:64:LEU:HG	4	0.01	0.01
(1,266)	1:A:41:VAL:HG22	1:B:64:LEU:HG	4	0.01	0.01
(1,266)	1:A:41:VAL:HG23	1:B:64:LEU:HG	4	0.01	0.01
(1,896)	1:A:53:ARG:HA	1:A:56:VAL:HB	3	0.01	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD2	3	0.01	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD3	3	0.01	0.01
(1,86)	1:B:23:LEU:N	1:B:19:LEU:O	3	0.01	0.01
(1,84)	1:B:22:VAL:N	1:B:18:ASP:O	3	0.01	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE21	3	0.01	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE22	3	0.01	0.01
(1,831)	1:A:46:ALA:HA	1:A:53:ARG:HE	3	0.01	0.02
(1,751)	1:A:39:ASN:HB2	1:A:42:THR:H	3	0.01	0.01
(1,751)	1:A:39:ASN:HB3	1:A:42:THR:H	3	0.01	0.01
(1,631)	1:A:23:LEU:H	1:A:26:GLU:H	3	0.01	0.02
(1,63)	1:A:69:LEU:N	1:A:65:LYS:O	3	0.01	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG21	3	0.01	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG22	3	0.01	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG23	3	0.01	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG21	3	0.01	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG22	3	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG23	3	0.01	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD2	3	0.01	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD3	3	0.01	0.01
(1,29)	1:A:35:MET:N	1:A:31:ASP:O	3	0.01	0.01
(1,23)	1:A:23:LEU:N	1:A:19:LEU:O	3	0.01	0.01
(1,21)	1:A:22:VAL:N	1:A:18:ASP:O	3	0.01	0.01
(1,1505)	1:B:70:GLU:HA	1:B:71:HIS:H	3	0.01	0.01
(1,1454)	1:B:59:ASN:HB2	1:B:63:ALA:H	3	0.02	0.02
(1,1454)	1:B:59:ASN:HB3	1:B:63:ALA:H	3	0.02	0.02
(1,1428)	1:B:56:VAL:HA	1:B:59:ASN:HD22	3	0.01	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD2	3	0.01	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD3	3	0.01	0.01
(1,1384)	1:B:50:GLU:HG2	1:B:53:ARG:H	3	0.01	0.01
(1,1384)	1:B:50:GLU:HG3	1:B:53:ARG:H	3	0.01	0.01
(1,13)	1:A:18:ASP:N	1:A:14:LYS:O	3	0.01	0.01
(1,118)	1:B:65:LYS:N	1:B:61:THR:O	3	0.01	0.01
(1,1138)	1:B:23:LEU:H	1:B:26:GLU:H	3	0.01	0.01
(1,876)	1:A:50:GLU:HG2	1:A:53:ARG:HE	2	0.01	0.01
(1,876)	1:A:50:GLU:HG3	1:A:53:ARG:HE	2	0.01	0.01
(1,868)	1:A:50:GLU:HA	1:A:53:ARG:HB3	2	0.01	0.01
(1,844)	1:A:48:VAL:HB	1:A:49:PRO:HD3	2	0.01	0.01
(1,819)	1:A:45:ILE:HG21	1:A:53:ARG:HG3	2	0.01	0.01
(1,819)	1:A:45:ILE:HG22	1:A:53:ARG:HG3	2	0.01	0.01
(1,819)	1:A:45:ILE:HG23	1:A:53:ARG:HG3	2	0.01	0.01
(1,76)	1:B:18:ASP:N	1:B:14:LYS:O	2	0.01	0.01
(1,669)	1:A:29:THR:HG21	1:A:30:PRO:HD2	2	0.01	0.01
(1,669)	1:A:29:THR:HG22	1:A:30:PRO:HD2	2	0.01	0.01
(1,669)	1:A:29:THR:HG23	1:A:30:PRO:HD2	2	0.01	0.01
(1,553)	1:A:14:LYS:HG2	1:A:18:ASP:H	2	0.01	0.02
(1,553)	1:A:14:LYS:HG3	1:A:18:ASP:H	2	0.01	0.02
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD21	2	0.01	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD22	2	0.01	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD23	2	0.01	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG21	2	0.01	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG22	2	0.01	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG23	2	0.01	0.01
(1,40)	1:A:58:ASP:H	1:A:54:VAL:O	2	0.01	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG21	2	0.01	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG22	2	0.01	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG23	2	0.01	0.01
(1,19)	1:A:21:ASP:N	1:A:17:GLN:O	2	0.01	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG21	2	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG22	2	0.01	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG23	2	0.01	0.01
(1,1403)	1:B:53:ARG:HA	1:B:56:VAL:HB	2	0.01	0.01
(1,1365)	1:B:49:PRO:HA	1:B:53:ARG:HE	2	0.01	0.02
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG2	2	0.01	0.02
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG3	2	0.01	0.02
(1,1353)	1:B:48:VAL:HB	1:B:53:ARG:HE	2	0.01	0.01
(1,1282)	1:B:41:VAL:H	1:B:42:THR:HB	2	0.01	0.01
(1,1234)	1:B:36:CYS:HB2	1:B:39:ASN:H	2	0.01	0.01
(1,1234)	1:B:36:CYS:HB3	1:B:39:ASN:H	2	0.01	0.01
(1,120)	1:B:66:GLN:N	1:B:62:LYS:O	2	0.01	0.01
(1,1186)	1:B:30:PRO:HB2	1:B:33:ALA:H	2	0.01	0.01
(1,1186)	1:B:30:PRO:HB3	1:B:33:ALA:H	2	0.01	0.01
(1,1133)	1:B:23:LEU:HD21	1:B:28:VAL:H	2	0.01	0.02
(1,1133)	1:B:23:LEU:HD22	1:B:28:VAL:H	2	0.01	0.02
(1,1133)	1:B:23:LEU:HD23	1:B:28:VAL:H	2	0.01	0.02
(1,1084)	1:B:17:GLN:HE22	1:B:20:LEU:HB3	2	0.01	0.01
(1,104)	1:B:58:ASP:N	1:B:54:VAL:O	2	0.01	0.01
(1,992)	1:A:66:GLN:HA	1:A:70:GLU:H	1	0.01	0.01
(1,921)	1:A:56:VAL:HA	1:A:59:ASN:HD22	1	0.01	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG21	1	0.01	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG22	1	0.01	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG23	1	0.01	0.01
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG21	1	0.01	0.01
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG22	1	0.01	0.01
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG23	1	0.01	0.01
(1,870)	1:A:50:GLU:HA	1:A:53:ARG:HD3	1	0.01	0.01
(1,869)	1:A:50:GLU:HA	1:A:53:ARG:HB2	1	0.01	0.01
(1,851)	1:A:48:VAL:HG11	1:A:53:ARG:HG2	1	0.01	0.01
(1,851)	1:A:48:VAL:HG11	1:A:53:ARG:HG3	1	0.01	0.01
(1,851)	1:A:48:VAL:HG12	1:A:53:ARG:HG2	1	0.01	0.01
(1,851)	1:A:48:VAL:HG12	1:A:53:ARG:HG3	1	0.01	0.01
(1,851)	1:A:48:VAL:HG13	1:A:53:ARG:HG2	1	0.01	0.01
(1,851)	1:A:48:VAL:HG13	1:A:53:ARG:HG3	1	0.01	0.01
(1,85)	1:B:23:LEU:H	1:B:19:LEU:O	1	0.01	0.01
(1,82)	1:B:21:ASP:N	1:B:17:GLN:O	1	0.01	0.01
(1,775)	1:A:41:VAL:H	1:A:42:THR:HB	1	0.01	0.01
(1,72)	1:B:16:ILE:N	1:B:12:VAL:O	1	0.01	0.01
(1,679)	1:A:30:PRO:HB2	1:A:33:ALA:H	1	0.01	0.01
(1,679)	1:A:30:PRO:HB3	1:A:33:ALA:H	1	0.01	0.01
(1,677)	1:A:30:PRO:HB2	1:A:32:LEU:H	1	0.01	0.01
(1,677)	1:A:30:PRO:HB3	1:A:32:LEU:H	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,67)	1:B:14:LYS:H	1:B:10:GLU:O	1	0.01	0.01
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG21	1	0.03	0.03
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG22	1	0.03	0.03
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG23	1	0.03	0.03
(1,638)	1:A:25:LYS:HA	1:A:27:GLU:HG2	1	0.01	0.01
(1,638)	1:A:25:LYS:HA	1:A:27:GLU:HG3	1	0.01	0.01
(1,635)	1:A:24:VAL:HG11	1:A:26:GLU:H	1	0.01	0.01
(1,635)	1:A:24:VAL:HG12	1:A:26:GLU:H	1	0.01	0.01
(1,635)	1:A:24:VAL:HG13	1:A:26:GLU:H	1	0.01	0.01
(1,62)	1:A:69:LEU:H	1:A:65:LYS:O	1	0.01	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG11	1	0.01	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG12	1	0.01	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG13	1	0.01	0.01
(1,60)	1:A:68:VAL:H	1:A:64:LEU:O	1	0.01	0.01
(1,577)	1:A:17:GLN:HE22	1:A:20:LEU:HB3	1	0.01	0.01
(1,576)	1:A:17:GLN:HE21	1:A:21:ASP:H	1	0.01	0.01
(1,576)	1:A:17:GLN:HE22	1:A:21:ASP:H	1	0.01	0.01
(1,524)	1:A:10:GLU:H	1:A:13:GLU:H	1	0.01	0.01
(1,499)	1:A:7:TYR:HD1	1:A:11:ARG:HD2	1	0.01	0.01
(1,499)	1:A:7:TYR:HD1	1:A:11:ARG:HD3	1	0.01	0.01
(1,499)	1:A:7:TYR:HD2	1:A:11:ARG:HD2	1	0.01	0.01
(1,499)	1:A:7:TYR:HD2	1:A:11:ARG:HD3	1	0.01	0.01
(1,494)	1:A:5:SER:HB2	1:A:7:TYR:H	1	0.02	0.02
(1,494)	1:A:5:SER:HB3	1:A:7:TYR:H	1	0.02	0.02
(1,49)	1:A:62:LYS:N	1:A:58:ASP:O	1	0.01	0.01
(1,476)	1:B:58:ASP:HA	1:A:65:LYS:HD2	1	0.01	0.01
(1,476)	1:B:58:ASP:HA	1:A:65:LYS:HD3	1	0.01	0.01
(1,467)	1:B:54:VAL:HG21	1:A:69:LEU:HA	1	0.01	0.01
(1,467)	1:B:54:VAL:HG22	1:A:69:LEU:HA	1	0.01	0.01
(1,467)	1:B:54:VAL:HG23	1:A:69:LEU:HA	1	0.01	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG21	1	0.01	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG22	1	0.01	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG23	1	0.01	0.01
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG11	1	0.01	0.01
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG12	1	0.01	0.01
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG13	1	0.01	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG11	1	0.01	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG12	1	0.01	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG13	1	0.01	0.01
(1,356)	1:B:16:ILE:HG12	1:A:36:CYS:HA	1	0.01	0.01
(1,341)	1:B:15:ILE:HG12	1:A:26:GLU:HG2	1	0.01	0.01
(1,341)	1:B:15:ILE:HG12	1:A:26:GLU:HG3	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,341)	1:B:15:ILE:HG13	1:A:26:GLU:HG2	1	0.01	0.01
(1,341)	1:B:15:ILE:HG13	1:A:26:GLU:HG3	1	0.01	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG11	1	0.01	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG12	1	0.01	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG13	1	0.01	0.01
(1,315)	1:B:7:TYR:HE1	1:A:29:THR:HB	1	0.01	0.01
(1,315)	1:B:7:TYR:HE2	1:A:29:THR:HB	1	0.01	0.01
(1,308)	1:A:61:THR:HG21	1:B:65:LYS:HG2	1	0.01	0.01
(1,308)	1:A:61:THR:HG21	1:B:65:LYS:HG3	1	0.01	0.01
(1,308)	1:A:61:THR:HG22	1:B:65:LYS:HG2	1	0.01	0.01
(1,308)	1:A:61:THR:HG22	1:B:65:LYS:HG3	1	0.01	0.01
(1,308)	1:A:61:THR:HG23	1:B:65:LYS:HG2	1	0.01	0.01
(1,308)	1:A:61:THR:HG23	1:B:65:LYS:HG3	1	0.01	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD11	1	0.01	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD12	1	0.01	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD13	1	0.01	0.01
(1,3)	1:A:13:GLU:H	1:A:9:ASN:C	1	0.01	0.01
(1,285)	1:A:54:VAL:HG21	1:B:69:LEU:HG	1	0.01	0.01
(1,285)	1:A:54:VAL:HG22	1:B:69:LEU:HG	1	0.01	0.01
(1,285)	1:A:54:VAL:HG23	1:B:69:LEU:HG	1	0.01	0.01
(1,284)	1:A:54:VAL:HG21	1:B:69:LEU:HA	1	0.01	0.01
(1,284)	1:A:54:VAL:HG22	1:B:69:LEU:HA	1	0.01	0.01
(1,284)	1:A:54:VAL:HG23	1:B:69:LEU:HA	1	0.01	0.01
(1,272)	1:A:42:THR:HG21	1:B:68:VAL:HA	1	0.01	0.01
(1,272)	1:A:42:THR:HG22	1:B:68:VAL:HA	1	0.01	0.01
(1,272)	1:A:42:THR:HG23	1:B:68:VAL:HA	1	0.01	0.01
(1,270)	1:A:42:THR:HG21	1:B:64:LEU:HA	1	0.01	0.01
(1,270)	1:A:42:THR:HG22	1:B:64:LEU:HA	1	0.01	0.01
(1,270)	1:A:42:THR:HG23	1:B:64:LEU:HA	1	0.01	0.01
(1,27)	1:A:25:LYS:N	1:A:21:ASP:O	1	0.01	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG21	1	0.01	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG22	1	0.01	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG23	1	0.01	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG21	1	0.01	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG22	1	0.01	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG23	1	0.01	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG21	1	0.01	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG22	1	0.01	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG23	1	0.01	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG21	1	0.01	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG22	1	0.01	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG23	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,22)	1:A:23:LEU:H	1:A:19:LEU:O	1	0.01	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD11	1	0.01	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD12	1	0.01	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD13	1	0.01	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD11	1	0.01	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD12	1	0.01	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD13	1	0.01	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD11	1	0.01	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD12	1	0.01	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD13	1	0.01	0.01
(1,20)	1:A:22:VAL:H	1:A:18:ASP:O	1	0.01	0.01
(1,158)	1:A:15:ILE:HG12	1:B:26:GLU:HG2	1	0.01	0.01
(1,158)	1:A:15:ILE:HG12	1:B:26:GLU:HG3	1	0.01	0.01
(1,158)	1:A:15:ILE:HG13	1:B:26:GLU:HG2	1	0.01	0.01
(1,158)	1:A:15:ILE:HG13	1:B:26:GLU:HG3	1	0.01	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG11	1	0.01	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG12	1	0.01	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG13	1	0.01	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG11	1	0.01	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG12	1	0.01	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG13	1	0.01	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG11	1	0.01	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG12	1	0.01	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG13	1	0.01	0.01
(1,1450)	1:B:59:ASN:HA	1:B:62:LYS:HD2	1	0.01	0.01
(1,1450)	1:B:59:ASN:HA	1:B:62:LYS:HD3	1	0.01	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD11	1	0.01	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD12	1	0.01	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD13	1	0.01	0.01
(1,1389)	1:B:50:GLU:H	1:B:53:ARG:HE	1	0.01	0.01
(1,1383)	1:B:50:GLU:HG2	1:B:53:ARG:HE	1	0.01	0.01
(1,1383)	1:B:50:GLU:HG3	1:B:53:ARG:HE	1	0.01	0.01
(1,1380)	1:B:50:GLU:HA	1:B:53:ARG:HG2	1	0.01	0.01
(1,1380)	1:B:50:GLU:HA	1:B:53:ARG:HG3	1	0.01	0.01
(1,1377)	1:B:50:GLU:HA	1:B:53:ARG:HD3	1	0.01	0.01
(1,1375)	1:B:50:GLU:HA	1:B:53:ARG:HB3	1	0.01	0.01
(1,1351)	1:B:48:VAL:HB	1:B:49:PRO:HD3	1	0.01	0.01
(1,1342)	1:B:46:ALA:H	1:B:47:GLN:HE21	1	0.01	0.01
(1,1342)	1:B:46:ALA:H	1:B:47:GLN:HE22	1	0.01	0.01
(1,1338)	1:B:46:ALA:HA	1:B:53:ARG:HE	1	0.01	0.01
(1,132)	1:A:7:TYR:HE1	1:B:29:THR:HB	1	0.01	0.01
(1,132)	1:A:7:TYR:HE2	1:B:29:THR:HB	1	0.01	0.01

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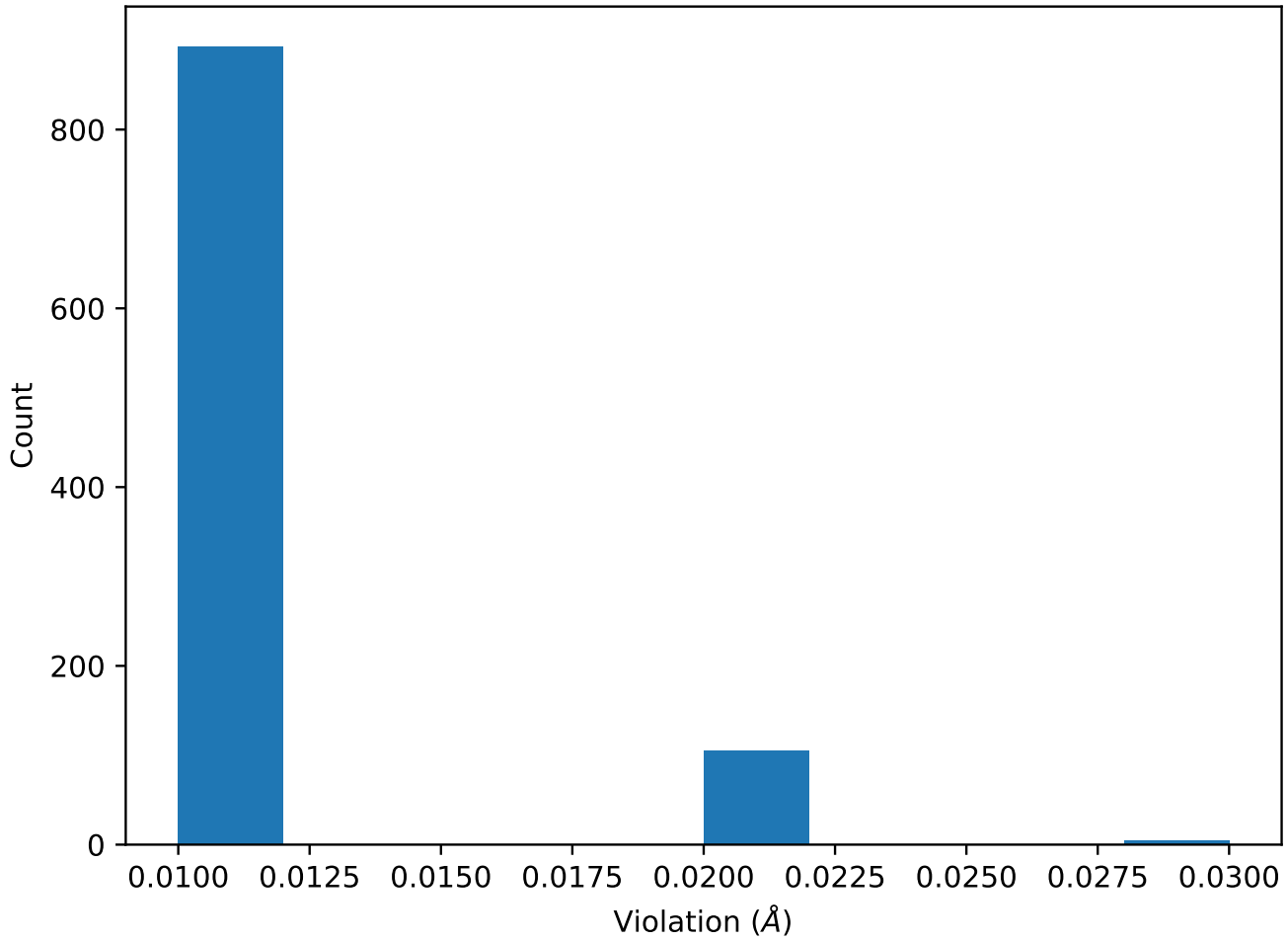
Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1311)	1:B:45:ILE:HD11	1:B:57:VAL:HB	1	0.01	0.01
(1,1311)	1:B:45:ILE:HD12	1:B:57:VAL:HB	1	0.01	0.01
(1,1311)	1:B:45:ILE:HD13	1:B:57:VAL:HB	1	0.01	0.01
(1,1298)	1:B:44:ILE:HD11	1:B:47:GLN:HE21	1	0.01	0.01
(1,1298)	1:B:44:ILE:HD12	1:B:47:GLN:HE21	1	0.01	0.01
(1,1298)	1:B:44:ILE:HD13	1:B:47:GLN:HE21	1	0.01	0.01
(1,126)	1:B:69:LEU:N	1:B:65:LYS:O	1	0.01	0.01
(1,125)	1:B:69:LEU:H	1:B:65:LYS:O	1	0.01	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD11	1	0.01	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD12	1	0.01	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD13	1	0.01	0.01
(1,1176)	1:B:29:THR:HG21	1:B:30:PRO:HD2	1	0.01	0.01
(1,1176)	1:B:29:THR:HG22	1:B:30:PRO:HD2	1	0.01	0.01
(1,1176)	1:B:29:THR:HG23	1:B:30:PRO:HD2	1	0.01	0.01
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG21	1	0.02	0.02
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG22	1	0.02	0.02
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG23	1	0.02	0.02
(1,1142)	1:B:24:VAL:HG11	1:B:26:GLU:H	1	0.01	0.01
(1,1142)	1:B:24:VAL:HG12	1:B:26:GLU:H	1	0.01	0.01
(1,1142)	1:B:24:VAL:HG13	1:B:26:GLU:H	1	0.01	0.01
(1,1131)	1:B:23:LEU:HD11	1:B:33:ALA:HA	1	0.01	0.01
(1,1131)	1:B:23:LEU:HD12	1:B:33:ALA:HA	1	0.01	0.01
(1,1131)	1:B:23:LEU:HD13	1:B:33:ALA:HA	1	0.01	0.01
(1,1123)	1:B:22:VAL:H	1:B:23:LEU:HB2	1	0.01	0.01
(1,1123)	1:B:22:VAL:H	1:B:23:LEU:HB3	1	0.01	0.01
(1,112)	1:B:62:LYS:N	1:B:58:ASP:O	1	0.01	0.01
(1,1119)	1:B:22:VAL:HA	1:B:25:LYS:HD2	1	0.01	0.01
(1,1119)	1:B:22:VAL:HA	1:B:25:LYS:HD3	1	0.01	0.01
(1,1083)	1:B:17:GLN:HE21	1:B:21:ASP:H	1	0.01	0.01
(1,1083)	1:B:17:GLN:HE22	1:B:21:ASP:H	1	0.01	0.01
(1,1060)	1:B:14:LYS:HG2	1:B:18:ASP:H	1	0.01	0.01
(1,1060)	1:B:14:LYS:HG3	1:B:18:ASP:H	1	0.01	0.01
(1,1031)	1:B:10:GLU:H	1:B:13:GLU:H	1	0.01	0.01
(1,103)	1:B:58:ASP:H	1:B:54:VAL:O	1	0.01	0.01
(1,1009)	1:B:8:SER:HA	1:B:11:ARG:HB2	1	0.01	0.01
(1,1009)	1:B:8:SER:HA	1:B:11:ARG:HB3	1	0.01	0.01

8.8 All distance violations

8.8.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of violations in the ensemble.



8.8.2 Table : All distance violations

The following table lists the violations in the ensemble sorted by violation value

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	19	0.03
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	19	0.03
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG21	6	0.03
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG22	6	0.03
(1,649)	1:A:28:VAL:HA	1:A:29:THR:HG23	6	0.03
(1,998)	1:A:70:GLU:HA	1:A:71:HIS:H	8	0.02
(1,998)	1:A:70:GLU:HA	1:A:71:HIS:H	10	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	1	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	1	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	2	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	2	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	4	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	4	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	5	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	5	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	6	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	6	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	12	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	12	0.02
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	14	0.02
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	14	0.02
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	5	0.02
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	5	0.02
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	4	0.02
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	18	0.02
(1,831)	1:A:46:ALA:HA	1:A:53:ARG:HE	19	0.02
(1,631)	1:A:23:LEU:H	1:A:26:GLU:H	19	0.02
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	16	0.02
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	16	0.02
(1,57)	1:A:66:GLN:N	1:A:62:LYS:O	11	0.02
(1,57)	1:A:66:GLN:N	1:A:62:LYS:O	13	0.02
(1,553)	1:A:14:LYS:HG2	1:A:18:ASP:H	17	0.02
(1,553)	1:A:14:LYS:HG3	1:A:18:ASP:H	17	0.02
(1,494)	1:A:5:SER:HB2	1:A:7:TYR:H	2	0.02
(1,494)	1:A:5:SER:HB3	1:A:7:TYR:H	2	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	12	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	12	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	12	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	12	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	12	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	12	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	14	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	14	0.02
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	14	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	14	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	14	0.02
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	14	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	1	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	1	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	1	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	1	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	1	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	1	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	3	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	3	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	3	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	3	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	3	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	3	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	6	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	6	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	6	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	6	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	6	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	6	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	12	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	12	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	12	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	12	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	12	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	12	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	15	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	15	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	15	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	15	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	15	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	15	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	18	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	18	0.02
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	18	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	18	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	18	0.02
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	18	0.02
(1,1454)	1:B:59:ASN:HB2	1:B:63:ALA:H	8	0.02
(1,1454)	1:B:59:ASN:HB3	1:B:63:ALA:H	8	0.02
(1,1454)	1:B:59:ASN:HB2	1:B:63:ALA:H	18	0.02
(1,1454)	1:B:59:ASN:HB3	1:B:63:ALA:H	18	0.02
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	1	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	1	0.02
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	9	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	9	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	12	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	12	0.02
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	16	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	16	0.02
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	19	0.02
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	19	0.02
(1,1365)	1:B:49:PRO:HA	1:B:53:ARG:HE	20	0.02
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG2	15	0.02
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG3	15	0.02
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	5	0.02
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	5	0.02
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG21	4	0.02
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG22	4	0.02
(1,1156)	1:B:28:VAL:HA	1:B:29:THR:HG23	4	0.02
(1,1133)	1:B:23:LEU:HD21	1:B:28:VAL:H	16	0.02
(1,1133)	1:B:23:LEU:HD22	1:B:28:VAL:H	16	0.02
(1,1133)	1:B:23:LEU:HD23	1:B:28:VAL:H	16	0.02
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	20	0.02
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	20	0.02
(1,998)	1:A:70:GLU:HA	1:A:71:HIS:H	1	0.01
(1,998)	1:A:70:GLU:HA	1:A:71:HIS:H	6	0.01
(1,992)	1:A:66:GLN:HA	1:A:70:GLU:H	19	0.01
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	3	0.01
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	3	0.01
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	8	0.01
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	8	0.01
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	15	0.01
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	15	0.01
(1,938)	1:A:58:ASP:HB2	1:A:62:LYS:H	17	0.01
(1,938)	1:A:58:ASP:HB3	1:A:62:LYS:H	17	0.01
(1,921)	1:A:56:VAL:HA	1:A:59:ASN:HD22	19	0.01
(1,90)	1:B:25:LYS:N	1:B:21:ASP:O	6	0.01
(1,90)	1:B:25:LYS:N	1:B:21:ASP:O	10	0.01
(1,90)	1:B:25:LYS:N	1:B:21:ASP:O	16	0.01
(1,90)	1:B:25:LYS:N	1:B:21:ASP:O	17	0.01
(1,896)	1:A:53:ARG:HA	1:A:56:VAL:HB	6	0.01
(1,896)	1:A:53:ARG:HA	1:A:56:VAL:HB	11	0.01
(1,896)	1:A:53:ARG:HA	1:A:56:VAL:HB	16	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG21	2	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG22	2	0.01
(1,893)	1:A:52:LYS:HG2	1:A:56:VAL:HG23	2	0.01
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG21	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG22	2	0.01
(1,893)	1:A:52:LYS:HG3	1:A:56:VAL:HG23	2	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD2	1	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD3	1	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD2	6	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD3	6	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD2	19	0.01
(1,881)	1:A:50:GLU:H	1:A:53:ARG:HD3	19	0.01
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	10	0.01
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	10	0.01
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	15	0.01
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	15	0.01
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	16	0.01
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	16	0.01
(1,877)	1:A:50:GLU:HG2	1:A:53:ARG:H	17	0.01
(1,877)	1:A:50:GLU:HG3	1:A:53:ARG:H	17	0.01
(1,876)	1:A:50:GLU:HG2	1:A:53:ARG:HE	1	0.01
(1,876)	1:A:50:GLU:HG3	1:A:53:ARG:HE	1	0.01
(1,876)	1:A:50:GLU:HG2	1:A:53:ARG:HE	3	0.01
(1,876)	1:A:50:GLU:HG3	1:A:53:ARG:HE	3	0.01
(1,870)	1:A:50:GLU:HA	1:A:53:ARG:HD3	19	0.01
(1,869)	1:A:50:GLU:HA	1:A:53:ARG:HB2	3	0.01
(1,868)	1:A:50:GLU:HA	1:A:53:ARG:HB3	2	0.01
(1,868)	1:A:50:GLU:HA	1:A:53:ARG:HB3	16	0.01
(1,86)	1:B:23:LEU:N	1:B:19:LEU:O	3	0.01
(1,86)	1:B:23:LEU:N	1:B:19:LEU:O	11	0.01
(1,86)	1:B:23:LEU:N	1:B:19:LEU:O	18	0.01
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	6	0.01
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	8	0.01
(1,858)	1:A:49:PRO:HA	1:A:53:ARG:HE	14	0.01
(1,851)	1:A:48:VAL:HG11	1:A:53:ARG:HG2	2	0.01
(1,851)	1:A:48:VAL:HG11	1:A:53:ARG:HG3	2	0.01
(1,851)	1:A:48:VAL:HG12	1:A:53:ARG:HG2	2	0.01
(1,851)	1:A:48:VAL:HG12	1:A:53:ARG:HG3	2	0.01
(1,851)	1:A:48:VAL:HG13	1:A:53:ARG:HG2	2	0.01
(1,851)	1:A:48:VAL:HG13	1:A:53:ARG:HG3	2	0.01
(1,85)	1:B:23:LEU:H	1:B:19:LEU:O	13	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	2	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	4	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	6	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	9	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	18	0.01
(1,846)	1:A:48:VAL:HB	1:A:53:ARG:HE	19	0.01
(1,844)	1:A:48:VAL:HB	1:A:49:PRO:HD3	10	0.01
(1,844)	1:A:48:VAL:HB	1:A:49:PRO:HD3	11	0.01
(1,84)	1:B:22:VAL:N	1:B:18:ASP:O	3	0.01
(1,84)	1:B:22:VAL:N	1:B:18:ASP:O	12	0.01
(1,84)	1:B:22:VAL:N	1:B:18:ASP:O	15	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE21	8	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE22	8	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE21	12	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE22	12	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE21	17	0.01
(1,835)	1:A:46:ALA:H	1:A:47:GLN:HE22	17	0.01
(1,831)	1:A:46:ALA:HA	1:A:53:ARG:HE	8	0.01
(1,831)	1:A:46:ALA:HA	1:A:53:ARG:HE	15	0.01
(1,82)	1:B:21:ASP:N	1:B:17:GLN:O	20	0.01
(1,819)	1:A:45:ILE:HG21	1:A:53:ARG:HG3	3	0.01
(1,819)	1:A:45:ILE:HG22	1:A:53:ARG:HG3	3	0.01
(1,819)	1:A:45:ILE:HG23	1:A:53:ARG:HG3	3	0.01
(1,819)	1:A:45:ILE:HG21	1:A:53:ARG:HG3	9	0.01
(1,819)	1:A:45:ILE:HG22	1:A:53:ARG:HG3	9	0.01
(1,819)	1:A:45:ILE:HG23	1:A:53:ARG:HG3	9	0.01
(1,775)	1:A:41:VAL:H	1:A:42:THR:HB	5	0.01
(1,76)	1:B:18:ASP:N	1:B:14:LYS:O	10	0.01
(1,76)	1:B:18:ASP:N	1:B:14:LYS:O	20	0.01
(1,751)	1:A:39:ASN:HB2	1:A:42:THR:H	5	0.01
(1,751)	1:A:39:ASN:HB3	1:A:42:THR:H	5	0.01
(1,751)	1:A:39:ASN:HB2	1:A:42:THR:H	11	0.01
(1,751)	1:A:39:ASN:HB3	1:A:42:THR:H	11	0.01
(1,751)	1:A:39:ASN:HB2	1:A:42:THR:H	17	0.01
(1,751)	1:A:39:ASN:HB3	1:A:42:THR:H	17	0.01
(1,72)	1:B:16:ILE:N	1:B:12:VAL:O	13	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	4	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	4	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	5	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	5	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	6	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	6	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	11	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	11	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	15	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	18	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	18	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD21	20	0.01
(1,714)	1:A:35:MET:HA	1:A:39:ASN:HD22	20	0.01
(1,679)	1:A:30:PRO:HB2	1:A:33:ALA:H	1	0.01
(1,679)	1:A:30:PRO:HB3	1:A:33:ALA:H	1	0.01
(1,677)	1:A:30:PRO:HB2	1:A:32:LEU:H	4	0.01
(1,677)	1:A:30:PRO:HB3	1:A:32:LEU:H	4	0.01
(1,67)	1:B:14:LYS:H	1:B:10:GLU:O	12	0.01
(1,669)	1:A:29:THR:HG21	1:A:30:PRO:HD2	6	0.01
(1,669)	1:A:29:THR:HG22	1:A:30:PRO:HD2	6	0.01
(1,669)	1:A:29:THR:HG23	1:A:30:PRO:HD2	6	0.01
(1,669)	1:A:29:THR:HG21	1:A:30:PRO:HD2	10	0.01
(1,669)	1:A:29:THR:HG22	1:A:30:PRO:HD2	10	0.01
(1,669)	1:A:29:THR:HG23	1:A:30:PRO:HD2	10	0.01
(1,646)	1:A:26:GLU:HG2	1:A:28:VAL:H	2	0.01
(1,646)	1:A:26:GLU:HG3	1:A:28:VAL:H	2	0.01
(1,646)	1:A:26:GLU:HG2	1:A:28:VAL:H	3	0.01
(1,646)	1:A:26:GLU:HG3	1:A:28:VAL:H	3	0.01
(1,646)	1:A:26:GLU:HG2	1:A:28:VAL:H	7	0.01
(1,646)	1:A:26:GLU:HG3	1:A:28:VAL:H	7	0.01
(1,646)	1:A:26:GLU:HG2	1:A:28:VAL:H	8	0.01
(1,646)	1:A:26:GLU:HG3	1:A:28:VAL:H	8	0.01
(1,638)	1:A:25:LYS:HA	1:A:27:GLU:HG2	12	0.01
(1,638)	1:A:25:LYS:HA	1:A:27:GLU:HG3	12	0.01
(1,635)	1:A:24:VAL:HG11	1:A:26:GLU:H	7	0.01
(1,635)	1:A:24:VAL:HG12	1:A:26:GLU:H	7	0.01
(1,635)	1:A:24:VAL:HG13	1:A:26:GLU:H	7	0.01
(1,631)	1:A:23:LEU:H	1:A:26:GLU:H	14	0.01
(1,631)	1:A:23:LEU:H	1:A:26:GLU:H	15	0.01
(1,63)	1:A:69:LEU:N	1:A:65:LYS:O	1	0.01
(1,63)	1:A:69:LEU:N	1:A:65:LYS:O	3	0.01
(1,63)	1:A:69:LEU:N	1:A:65:LYS:O	16	0.01
(1,62)	1:A:69:LEU:H	1:A:65:LYS:O	17	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	5	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	5	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	6	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	6	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	11	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	11	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	14	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	17	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	17	0.01
(1,606)	1:A:21:ASP:HB2	1:A:25:LYS:H	19	0.01
(1,606)	1:A:21:ASP:HB3	1:A:25:LYS:H	19	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG11	19	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG12	19	0.01
(1,601)	1:A:21:ASP:HA	1:A:24:VAL:HG13	19	0.01
(1,60)	1:A:68:VAL:H	1:A:64:LEU:O	18	0.01
(1,577)	1:A:17:GLN:HE22	1:A:20:LEU:HB3	5	0.01
(1,576)	1:A:17:GLN:HE21	1:A:21:ASP:H	17	0.01
(1,576)	1:A:17:GLN:HE22	1:A:21:ASP:H	17	0.01
(1,57)	1:A:66:GLN:N	1:A:62:LYS:O	3	0.01
(1,57)	1:A:66:GLN:N	1:A:62:LYS:O	6	0.01
(1,553)	1:A:14:LYS:HG2	1:A:18:ASP:H	8	0.01
(1,553)	1:A:14:LYS:HG3	1:A:18:ASP:H	8	0.01
(1,55)	1:A:65:LYS:N	1:A:61:THR:O	1	0.01
(1,55)	1:A:65:LYS:N	1:A:61:THR:O	3	0.01
(1,55)	1:A:65:LYS:N	1:A:61:THR:O	8	0.01
(1,55)	1:A:65:LYS:N	1:A:61:THR:O	17	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG21	4	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG22	4	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG23	4	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG21	4	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG22	4	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG23	4	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG21	7	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG22	7	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG23	7	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG21	7	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG22	7	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG23	7	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG21	11	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG22	11	0.01
(1,532)	1:A:11:ARG:HG2	1:A:15:ILE:HG23	11	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG21	11	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG22	11	0.01
(1,532)	1:A:11:ARG:HG3	1:A:15:ILE:HG23	11	0.01
(1,524)	1:A:10:GLU:H	1:A:13:GLU:H	6	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG2	9	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG3	9	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG2	10	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG3	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG2	12	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG3	12	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG2	17	0.01
(1,509)	1:A:8:SER:H	1:A:11:ARG:HG3	17	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	2	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	2	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	2	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	2	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	2	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	2	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	4	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	4	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	4	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	4	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	4	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	4	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	10	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	10	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	10	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	10	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	10	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	10	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	11	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	11	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	11	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	11	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	11	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	11	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	13	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	13	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	13	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	13	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	13	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	13	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	20	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	20	0.01
(1,501)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	20	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	20	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	20	0.01
(1,501)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	20	0.01
(1,499)	1:A:7:TYR:HD1	1:A:11:ARG:HD2	12	0.01
(1,499)	1:A:7:TYR:HD1	1:A:11:ARG:HD3	12	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,499)	1:A:7:TYR:HD2	1:A:11:ARG:HD2	12	0.01
(1,499)	1:A:7:TYR:HD2	1:A:11:ARG:HD3	12	0.01
(1,49)	1:A:62:LYS:N	1:A:58:ASP:O	15	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD21	11	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD22	11	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD23	11	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD21	14	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD22	14	0.01
(1,485)	1:B:60:PHE:HZ	1:A:64:LEU:HD23	14	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	1	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	1	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	1	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	1	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	1	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	1	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	2	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	2	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	2	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	2	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	2	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	2	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	3	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	3	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	3	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	3	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	3	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	3	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	4	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	4	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	4	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	4	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	4	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	4	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	5	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	5	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	5	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	5	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	5	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	5	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	6	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	6	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	6	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	6	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	6	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	6	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	7	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	7	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	7	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	7	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	7	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	7	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	8	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	8	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	8	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	8	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	8	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	8	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	9	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	9	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	9	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	9	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	9	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	9	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	10	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	10	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	10	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	10	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	10	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	10	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	11	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	11	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	11	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	11	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	11	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	11	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	13	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	13	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	13	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	13	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	13	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	13	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	15	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	15	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	15	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	15	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	15	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	16	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	16	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	16	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	16	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	16	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	16	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	17	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	17	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	17	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	17	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	17	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	17	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	18	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	18	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	18	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	18	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	18	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	18	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	19	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	19	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	19	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	19	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	19	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	19	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG21	20	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG22	20	0.01
(1,478)	1:B:60:PHE:HB2	1:A:61:THR:HG23	20	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG21	20	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG22	20	0.01
(1,478)	1:B:60:PHE:HB3	1:A:61:THR:HG23	20	0.01
(1,476)	1:B:58:ASP:HA	1:A:65:LYS:HD2	17	0.01
(1,476)	1:B:58:ASP:HA	1:A:65:LYS:HD3	17	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	2	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	2	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	2	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	9	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	9	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	9	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	10	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	10	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	12	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	12	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	12	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	13	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	13	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	13	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	19	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	19	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	19	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD21	20	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD22	20	0.01
(1,469)	1:B:57:VAL:HB	1:A:64:LEU:HD23	20	0.01
(1,467)	1:B:54:VAL:HG21	1:A:69:LEU:HA	17	0.01
(1,467)	1:B:54:VAL:HG22	1:A:69:LEU:HA	17	0.01
(1,467)	1:B:54:VAL:HG23	1:A:69:LEU:HA	17	0.01
(1,449)	1:B:41:VAL:HG21	1:A:64:LEU:HG	1	0.01
(1,449)	1:B:41:VAL:HG22	1:A:64:LEU:HG	1	0.01
(1,449)	1:B:41:VAL:HG23	1:A:64:LEU:HG	1	0.01
(1,449)	1:B:41:VAL:HG21	1:A:64:LEU:HG	7	0.01
(1,449)	1:B:41:VAL:HG22	1:A:64:LEU:HG	7	0.01
(1,449)	1:B:41:VAL:HG23	1:A:64:LEU:HG	7	0.01
(1,449)	1:B:41:VAL:HG21	1:A:64:LEU:HG	8	0.01
(1,449)	1:B:41:VAL:HG22	1:A:64:LEU:HG	8	0.01
(1,449)	1:B:41:VAL:HG23	1:A:64:LEU:HG	8	0.01
(1,449)	1:B:41:VAL:HG21	1:A:64:LEU:HG	20	0.01
(1,449)	1:B:41:VAL:HG22	1:A:64:LEU:HG	20	0.01
(1,449)	1:B:41:VAL:HG23	1:A:64:LEU:HG	20	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG21	7	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG22	7	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG23	7	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG21	16	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG22	16	0.01
(1,410)	1:B:33:ALA:H	1:A:44:ILE:HG23	16	0.01
(1,41)	1:A:58:ASP:N	1:A:54:VAL:O	2	0.01
(1,41)	1:A:58:ASP:N	1:A:54:VAL:O	3	0.01
(1,41)	1:A:58:ASP:N	1:A:54:VAL:O	6	0.01
(1,41)	1:A:58:ASP:N	1:A:54:VAL:O	11	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG21	2	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG22	2	0.01
(1,405)	1:B:33:ALA:HA	1:A:44:ILE:HG23	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG11	14	0.01
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG12	14	0.01
(1,404)	1:B:30:PRO:HG2	1:A:48:VAL:HG13	14	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG11	14	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG12	14	0.01
(1,404)	1:B:30:PRO:HG3	1:A:48:VAL:HG13	14	0.01
(1,40)	1:A:58:ASP:H	1:A:54:VAL:O	5	0.01
(1,40)	1:A:58:ASP:H	1:A:54:VAL:O	17	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG21	4	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG22	4	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG23	4	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG21	5	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG22	5	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG23	5	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG21	11	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG22	11	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG23	11	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG21	17	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG22	17	0.01
(1,366)	1:B:18:ASP:HA	1:A:22:VAL:HG23	17	0.01
(1,356)	1:B:16:ILE:HG12	1:A:36:CYS:HA	20	0.01
(1,341)	1:B:15:ILE:HG12	1:A:26:GLU:HG2	12	0.01
(1,341)	1:B:15:ILE:HG12	1:A:26:GLU:HG3	12	0.01
(1,341)	1:B:15:ILE:HG13	1:A:26:GLU:HG2	12	0.01
(1,341)	1:B:15:ILE:HG13	1:A:26:GLU:HG3	12	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG11	8	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG12	8	0.01
(1,321)	1:B:11:ARG:HE	1:A:28:VAL:HG13	8	0.01
(1,315)	1:B:7:TYR:HE1	1:A:29:THR:HB	16	0.01
(1,315)	1:B:7:TYR:HE2	1:A:29:THR:HB	16	0.01
(1,308)	1:A:61:THR:HG21	1:B:65:LYS:HG2	15	0.01
(1,308)	1:A:61:THR:HG21	1:B:65:LYS:HG3	15	0.01
(1,308)	1:A:61:THR:HG22	1:B:65:LYS:HG2	15	0.01
(1,308)	1:A:61:THR:HG22	1:B:65:LYS:HG3	15	0.01
(1,308)	1:A:61:THR:HG23	1:B:65:LYS:HG2	15	0.01
(1,308)	1:A:61:THR:HG23	1:B:65:LYS:HG3	15	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD11	4	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD12	4	0.01
(1,303)	1:A:61:THR:HA	1:B:64:LEU:HD13	4	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	1	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	1	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	1	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	4	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	4	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	4	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	12	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	12	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	12	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	15	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	15	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	15	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	17	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	17	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	17	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	18	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	18	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	18	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD21	19	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD22	19	0.01
(1,302)	1:A:60:PHE:HZ	1:B:64:LEU:HD23	19	0.01
(1,3)	1:A:13:GLU:H	1:A:9:ASN:C	2	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	2	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	2	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	2	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	2	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	2	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	2	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	4	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	4	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	4	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	4	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	4	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	4	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	5	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	5	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	5	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	5	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	5	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	5	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	7	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	7	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	7	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	7	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	7	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	8	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	8	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	8	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	8	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	8	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	8	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	9	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	9	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	9	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	9	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	9	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	9	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	10	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	10	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	10	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	10	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	10	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	10	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	11	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	11	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	11	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	11	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	11	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	11	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	13	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	13	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	13	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	13	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	13	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	13	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	14	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	14	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	14	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	14	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	14	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	14	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	16	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	16	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	16	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	16	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	16	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	16	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	17	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	17	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	17	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	17	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	17	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	17	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	19	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	19	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	19	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	19	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	19	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	19	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG21	20	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG22	20	0.01
(1,295)	1:A:60:PHE:HB2	1:B:61:THR:HG23	20	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG21	20	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG22	20	0.01
(1,295)	1:A:60:PHE:HB3	1:B:61:THR:HG23	20	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD2	9	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD3	9	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD2	13	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD3	13	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD2	19	0.01
(1,293)	1:A:58:ASP:HA	1:B:65:LYS:HD3	19	0.01
(1,29)	1:A:35:MET:N	1:A:31:ASP:O	4	0.01
(1,29)	1:A:35:MET:N	1:A:31:ASP:O	6	0.01
(1,29)	1:A:35:MET:N	1:A:31:ASP:O	11	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	2	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	2	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	2	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	3	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	3	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	3	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	8	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	8	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	8	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	10	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	10	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	10	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD21	14	0.01
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD22	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,286)	1:A:57:VAL:HB	1:B:64:LEU:HD23	14	0.01
(1,285)	1:A:54:VAL:HG21	1:B:69:LEU:HG	10	0.01
(1,285)	1:A:54:VAL:HG22	1:B:69:LEU:HG	10	0.01
(1,285)	1:A:54:VAL:HG23	1:B:69:LEU:HG	10	0.01
(1,284)	1:A:54:VAL:HG21	1:B:69:LEU:HA	8	0.01
(1,284)	1:A:54:VAL:HG22	1:B:69:LEU:HA	8	0.01
(1,284)	1:A:54:VAL:HG23	1:B:69:LEU:HA	8	0.01
(1,272)	1:A:42:THR:HG21	1:B:68:VAL:HA	5	0.01
(1,272)	1:A:42:THR:HG22	1:B:68:VAL:HA	5	0.01
(1,272)	1:A:42:THR:HG23	1:B:68:VAL:HA	5	0.01
(1,270)	1:A:42:THR:HG21	1:B:64:LEU:HA	5	0.01
(1,270)	1:A:42:THR:HG22	1:B:64:LEU:HA	5	0.01
(1,270)	1:A:42:THR:HG23	1:B:64:LEU:HA	5	0.01
(1,27)	1:A:25:LYS:N	1:A:21:ASP:O	2	0.01
(1,266)	1:A:41:VAL:HG21	1:B:64:LEU:HG	3	0.01
(1,266)	1:A:41:VAL:HG22	1:B:64:LEU:HG	3	0.01
(1,266)	1:A:41:VAL:HG23	1:B:64:LEU:HG	3	0.01
(1,266)	1:A:41:VAL:HG21	1:B:64:LEU:HG	7	0.01
(1,266)	1:A:41:VAL:HG22	1:B:64:LEU:HG	7	0.01
(1,266)	1:A:41:VAL:HG23	1:B:64:LEU:HG	7	0.01
(1,266)	1:A:41:VAL:HG21	1:B:64:LEU:HG	11	0.01
(1,266)	1:A:41:VAL:HG22	1:B:64:LEU:HG	11	0.01
(1,266)	1:A:41:VAL:HG23	1:B:64:LEU:HG	11	0.01
(1,266)	1:A:41:VAL:HG21	1:B:64:LEU:HG	20	0.01
(1,266)	1:A:41:VAL:HG22	1:B:64:LEU:HG	20	0.01
(1,266)	1:A:41:VAL:HG23	1:B:64:LEU:HG	20	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG21	13	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG22	13	0.01
(1,246)	1:A:37:LEU:HD11	1:B:41:VAL:HG23	13	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG21	13	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG22	13	0.01
(1,246)	1:A:37:LEU:HD12	1:B:41:VAL:HG23	13	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG21	13	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG22	13	0.01
(1,246)	1:A:37:LEU:HD13	1:B:41:VAL:HG23	13	0.01
(1,23)	1:A:23:LEU:N	1:A:19:LEU:O	4	0.01
(1,23)	1:A:23:LEU:N	1:A:19:LEU:O	11	0.01
(1,23)	1:A:23:LEU:N	1:A:19:LEU:O	20	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG21	4	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG22	4	0.01
(1,227)	1:A:33:ALA:H	1:B:44:ILE:HG23	4	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG21	5	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG22	5	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG23	5	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG21	15	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG22	15	0.01
(1,222)	1:A:33:ALA:HA	1:B:44:ILE:HG23	15	0.01
(1,22)	1:A:23:LEU:H	1:A:19:LEU:O	19	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD11	15	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD12	15	0.01
(1,212)	1:A:23:LEU:HD11	1:B:44:ILE:HD13	15	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD11	15	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD12	15	0.01
(1,212)	1:A:23:LEU:HD12	1:B:44:ILE:HD13	15	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD11	15	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD12	15	0.01
(1,212)	1:A:23:LEU:HD13	1:B:44:ILE:HD13	15	0.01
(1,21)	1:A:22:VAL:N	1:A:18:ASP:O	16	0.01
(1,21)	1:A:22:VAL:N	1:A:18:ASP:O	17	0.01
(1,21)	1:A:22:VAL:N	1:A:18:ASP:O	19	0.01
(1,20)	1:A:22:VAL:H	1:A:18:ASP:O	3	0.01
(1,19)	1:A:21:ASP:N	1:A:17:GLN:O	17	0.01
(1,19)	1:A:21:ASP:N	1:A:17:GLN:O	18	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG21	12	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG22	12	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG23	12	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG21	14	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG22	14	0.01
(1,183)	1:A:18:ASP:HA	1:B:22:VAL:HG23	14	0.01
(1,158)	1:A:15:ILE:HG12	1:B:26:GLU:HG2	7	0.01
(1,158)	1:A:15:ILE:HG12	1:B:26:GLU:HG3	7	0.01
(1,158)	1:A:15:ILE:HG13	1:B:26:GLU:HG2	7	0.01
(1,158)	1:A:15:ILE:HG13	1:B:26:GLU:HG3	7	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG11	14	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG12	14	0.01
(1,153)	1:A:15:ILE:HD11	1:B:28:VAL:HG13	14	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG11	14	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG12	14	0.01
(1,153)	1:A:15:ILE:HD12	1:B:28:VAL:HG13	14	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG11	14	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG12	14	0.01
(1,153)	1:A:15:ILE:HD13	1:B:28:VAL:HG13	14	0.01
(1,1505)	1:B:70:GLU:HA	1:B:71:HIS:H	7	0.01
(1,1505)	1:B:70:GLU:HA	1:B:71:HIS:H	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1505)	1:B:70:GLU:HA	1:B:71:HIS:H	20	0.01
(1,1454)	1:B:59:ASN:HB2	1:B:63:ALA:H	12	0.01
(1,1454)	1:B:59:ASN:HB3	1:B:63:ALA:H	12	0.01
(1,1450)	1:B:59:ASN:HA	1:B:62:LYS:HD2	16	0.01
(1,1450)	1:B:59:ASN:HA	1:B:62:LYS:HD3	16	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	2	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	2	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	3	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	3	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	4	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	4	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	5	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	5	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	6	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	6	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	7	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	7	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	8	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	8	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	10	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	10	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	11	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	11	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	15	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	15	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	18	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	18	0.01
(1,1445)	1:B:58:ASP:HB2	1:B:62:LYS:H	20	0.01
(1,1445)	1:B:58:ASP:HB3	1:B:62:LYS:H	20	0.01
(1,1428)	1:B:56:VAL:HA	1:B:59:ASN:HD22	5	0.01
(1,1428)	1:B:56:VAL:HA	1:B:59:ASN:HD22	12	0.01
(1,1428)	1:B:56:VAL:HA	1:B:59:ASN:HD22	18	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD11	13	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD12	13	0.01
(1,141)	1:A:12:VAL:H	1:B:32:LEU:HD13	13	0.01
(1,1403)	1:B:53:ARG:HA	1:B:56:VAL:HB	11	0.01
(1,1403)	1:B:53:ARG:HA	1:B:56:VAL:HB	17	0.01
(1,1389)	1:B:50:GLU:H	1:B:53:ARG:HE	17	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD2	7	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD3	7	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD2	15	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD3	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD2	18	0.01
(1,1388)	1:B:50:GLU:H	1:B:53:ARG:HD3	18	0.01
(1,1384)	1:B:50:GLU:HG2	1:B:53:ARG:H	8	0.01
(1,1384)	1:B:50:GLU:HG3	1:B:53:ARG:H	8	0.01
(1,1384)	1:B:50:GLU:HG2	1:B:53:ARG:H	11	0.01
(1,1384)	1:B:50:GLU:HG3	1:B:53:ARG:H	11	0.01
(1,1384)	1:B:50:GLU:HG2	1:B:53:ARG:H	18	0.01
(1,1384)	1:B:50:GLU:HG3	1:B:53:ARG:H	18	0.01
(1,1383)	1:B:50:GLU:HG2	1:B:53:ARG:HE	17	0.01
(1,1383)	1:B:50:GLU:HG3	1:B:53:ARG:HE	17	0.01
(1,1380)	1:B:50:GLU:HA	1:B:53:ARG:HG2	15	0.01
(1,1380)	1:B:50:GLU:HA	1:B:53:ARG:HG3	15	0.01
(1,1377)	1:B:50:GLU:HA	1:B:53:ARG:HD3	17	0.01
(1,1375)	1:B:50:GLU:HA	1:B:53:ARG:HB3	13	0.01
(1,1365)	1:B:49:PRO:HA	1:B:53:ARG:HE	17	0.01
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG2	17	0.01
(1,1364)	1:B:48:VAL:H	1:B:53:ARG:HG3	17	0.01
(1,1353)	1:B:48:VAL:HB	1:B:53:ARG:HE	6	0.01
(1,1353)	1:B:48:VAL:HB	1:B:53:ARG:HE	20	0.01
(1,1351)	1:B:48:VAL:HB	1:B:49:PRO:HD3	1	0.01
(1,1342)	1:B:46:ALA:H	1:B:47:GLN:HE21	1	0.01
(1,1342)	1:B:46:ALA:H	1:B:47:GLN:HE22	1	0.01
(1,1338)	1:B:46:ALA:HA	1:B:53:ARG:HE	20	0.01
(1,132)	1:A:7:TYR:HE1	1:B:29:THR:HB	13	0.01
(1,132)	1:A:7:TYR:HE2	1:B:29:THR:HB	13	0.01
(1,1311)	1:B:45:ILE:HD11	1:B:57:VAL:HB	1	0.01
(1,1311)	1:B:45:ILE:HD12	1:B:57:VAL:HB	1	0.01
(1,1311)	1:B:45:ILE:HD13	1:B:57:VAL:HB	1	0.01
(1,13)	1:A:18:ASP:N	1:A:14:LYS:O	3	0.01
(1,13)	1:A:18:ASP:N	1:A:14:LYS:O	10	0.01
(1,13)	1:A:18:ASP:N	1:A:14:LYS:O	17	0.01
(1,1298)	1:B:44:ILE:HD11	1:B:47:GLN:HE21	15	0.01
(1,1298)	1:B:44:ILE:HD12	1:B:47:GLN:HE21	15	0.01
(1,1298)	1:B:44:ILE:HD13	1:B:47:GLN:HE21	15	0.01
(1,1282)	1:B:41:VAL:H	1:B:42:THR:HB	18	0.01
(1,1282)	1:B:41:VAL:H	1:B:42:THR:HB	19	0.01
(1,126)	1:B:69:LEU:N	1:B:65:LYS:O	8	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	7	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	7	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	8	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	8	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	9	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	12	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	12	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	13	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	13	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	19	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	19	0.01
(1,1258)	1:B:39:ASN:HB2	1:B:42:THR:H	20	0.01
(1,1258)	1:B:39:ASN:HB3	1:B:42:THR:H	20	0.01
(1,125)	1:B:69:LEU:H	1:B:65:LYS:O	7	0.01
(1,1234)	1:B:36:CYS:HB2	1:B:39:ASN:H	10	0.01
(1,1234)	1:B:36:CYS:HB3	1:B:39:ASN:H	10	0.01
(1,1234)	1:B:36:CYS:HB2	1:B:39:ASN:H	13	0.01
(1,1234)	1:B:36:CYS:HB3	1:B:39:ASN:H	13	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	7	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	7	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	8	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	8	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	10	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	10	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	13	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	13	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	14	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	14	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	17	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	17	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	19	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	19	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD21	20	0.01
(1,1221)	1:B:35:MET:HA	1:B:39:ASN:HD22	20	0.01
(1,120)	1:B:66:GLN:N	1:B:62:LYS:O	6	0.01
(1,120)	1:B:66:GLN:N	1:B:62:LYS:O	11	0.01
(1,1186)	1:B:30:PRO:HB2	1:B:33:ALA:H	7	0.01
(1,1186)	1:B:30:PRO:HB3	1:B:33:ALA:H	7	0.01
(1,1186)	1:B:30:PRO:HB2	1:B:33:ALA:H	9	0.01
(1,1186)	1:B:30:PRO:HB3	1:B:33:ALA:H	9	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD11	17	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD12	17	0.01
(1,1180)	1:B:29:THR:H	1:B:32:LEU:HD13	17	0.01
(1,118)	1:B:65:LYS:N	1:B:61:THR:O	1	0.01
(1,118)	1:B:65:LYS:N	1:B:61:THR:O	7	0.01
(1,118)	1:B:65:LYS:N	1:B:61:THR:O	19	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1176)	1:B:29:THR:HG21	1:B:30:PRO:HD2	4	0.01
(1,1176)	1:B:29:THR:HG22	1:B:30:PRO:HD2	4	0.01
(1,1176)	1:B:29:THR:HG23	1:B:30:PRO:HD2	4	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	4	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	4	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	6	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	6	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	8	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	8	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	14	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	14	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	16	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	16	0.01
(1,1153)	1:B:26:GLU:HG2	1:B:28:VAL:H	20	0.01
(1,1153)	1:B:26:GLU:HG3	1:B:28:VAL:H	20	0.01
(1,1142)	1:B:24:VAL:HG11	1:B:26:GLU:H	4	0.01
(1,1142)	1:B:24:VAL:HG12	1:B:26:GLU:H	4	0.01
(1,1142)	1:B:24:VAL:HG13	1:B:26:GLU:H	4	0.01
(1,1138)	1:B:23:LEU:H	1:B:26:GLU:H	1	0.01
(1,1138)	1:B:23:LEU:H	1:B:26:GLU:H	7	0.01
(1,1138)	1:B:23:LEU:H	1:B:26:GLU:H	13	0.01
(1,1133)	1:B:23:LEU:HD21	1:B:28:VAL:H	18	0.01
(1,1133)	1:B:23:LEU:HD22	1:B:28:VAL:H	18	0.01
(1,1133)	1:B:23:LEU:HD23	1:B:28:VAL:H	18	0.01
(1,1131)	1:B:23:LEU:HD11	1:B:33:ALA:HA	16	0.01
(1,1131)	1:B:23:LEU:HD12	1:B:33:ALA:HA	16	0.01
(1,1131)	1:B:23:LEU:HD13	1:B:33:ALA:HA	16	0.01
(1,1123)	1:B:22:VAL:H	1:B:23:LEU:HB2	18	0.01
(1,1123)	1:B:22:VAL:H	1:B:23:LEU:HB3	18	0.01
(1,112)	1:B:62:LYS:N	1:B:58:ASP:O	2	0.01
(1,1119)	1:B:22:VAL:HA	1:B:25:LYS:HD2	7	0.01
(1,1119)	1:B:22:VAL:HA	1:B:25:LYS:HD3	7	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	3	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	3	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	6	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	6	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	8	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	8	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	10	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	10	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	11	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	11	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	12	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	12	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	15	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	15	0.01
(1,1113)	1:B:21:ASP:HB2	1:B:25:LYS:H	16	0.01
(1,1113)	1:B:21:ASP:HB3	1:B:25:LYS:H	16	0.01
(1,1084)	1:B:17:GLN:HE22	1:B:20:LEU:HB3	17	0.01
(1,1084)	1:B:17:GLN:HE22	1:B:20:LEU:HB3	20	0.01
(1,1083)	1:B:17:GLN:HE21	1:B:21:ASP:H	19	0.01
(1,1083)	1:B:17:GLN:HE22	1:B:21:ASP:H	19	0.01
(1,1060)	1:B:14:LYS:HG2	1:B:18:ASP:H	4	0.01
(1,1060)	1:B:14:LYS:HG3	1:B:18:ASP:H	4	0.01
(1,104)	1:B:58:ASP:N	1:B:54:VAL:O	10	0.01
(1,104)	1:B:58:ASP:N	1:B:54:VAL:O	20	0.01
(1,1031)	1:B:10:GLU:H	1:B:13:GLU:H	15	0.01
(1,103)	1:B:58:ASP:H	1:B:54:VAL:O	7	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	1	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	1	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	8	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	8	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	10	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	10	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	11	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	11	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	15	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	15	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG2	18	0.01
(1,1016)	1:B:8:SER:H	1:B:11:ARG:HG3	18	0.01
(1,1009)	1:B:8:SER:HA	1:B:11:ARG:HB2	12	0.01
(1,1009)	1:B:8:SER:HA	1:B:11:ARG:HB3	12	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	3	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	3	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	3	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	3	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	3	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	3	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	6	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	6	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	6	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	6	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	6	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	6	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	8	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	8	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	8	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	8	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	8	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	8	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	9	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	9	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	9	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	9	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	9	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	9	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	13	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	13	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	13	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	13	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	13	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	13	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	15	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	15	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	15	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	15	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	15	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	15	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	16	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	16	0.01
(1,1008)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	16	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	16	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	16	0.01
(1,1008)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	16	0.01

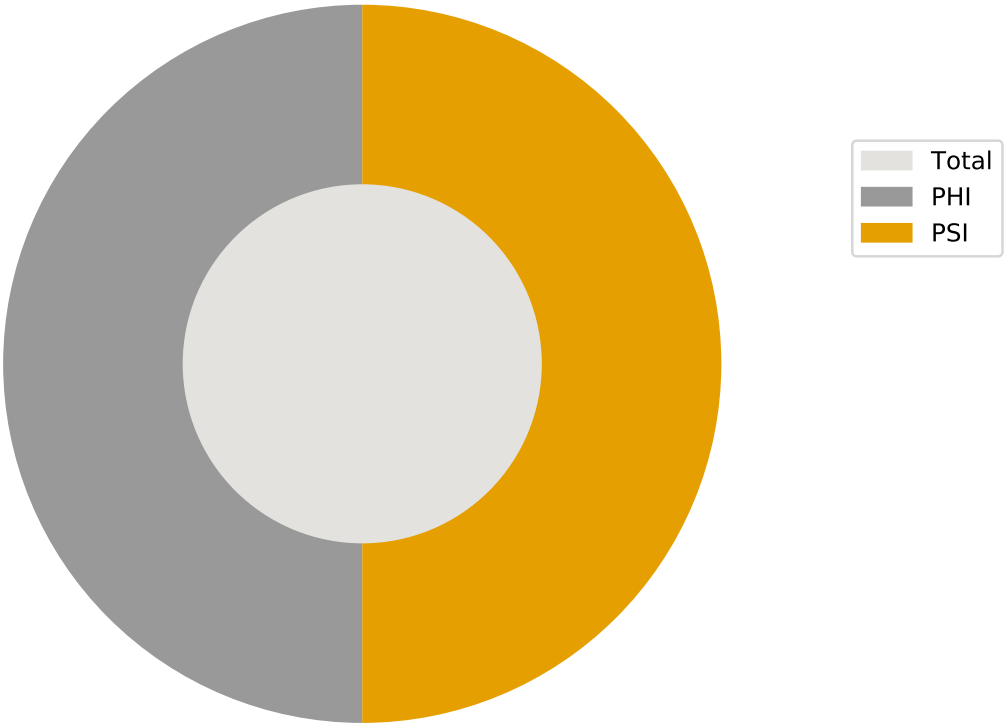
9 Dihedral angle restraints analysis

9.1 Dihedral angle restraints summary

Angle name	Count	%
PHI	106	50.0
PSI	106	50.0
Total	212	100.0

9.1.1 Pie chart : Dihedral angle restraints

There are 0 unmapped restraints



9.2 Dihedral angle violations

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

Angle name	Count	%[1]	%[2]
PHI	0	0.0	0.0
PSI	0	0.0	0.0

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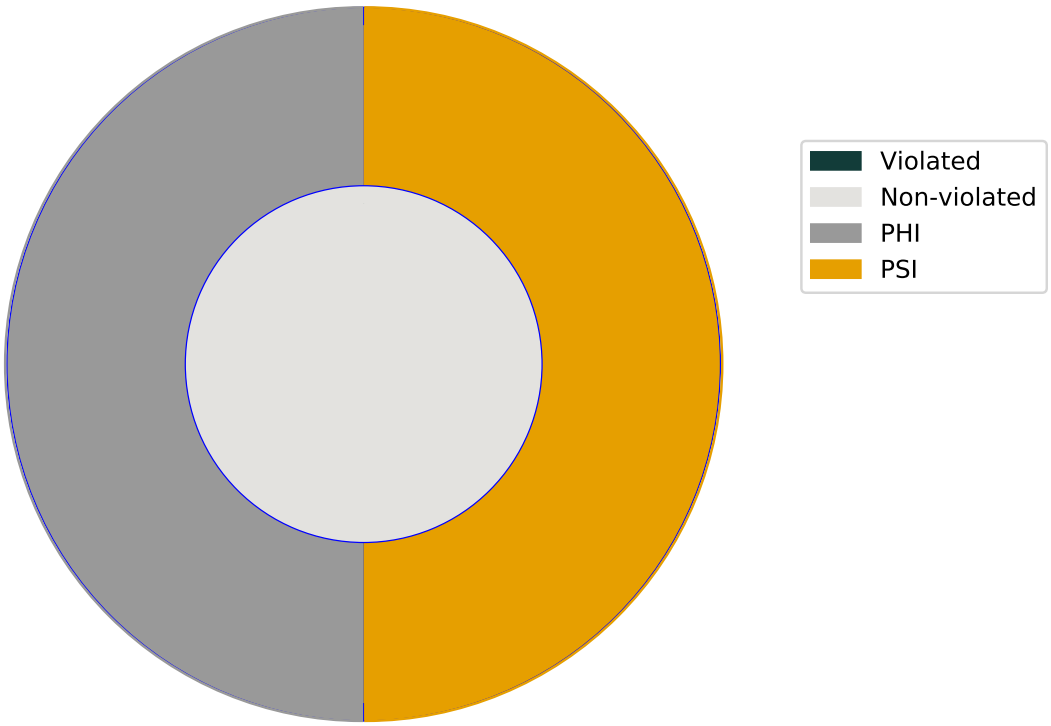
Angle name	Count	%[1]	%[2]
Total	0	0.0	0.0

[1]percentage of violated restraints in that particular angle type, [2]percentage of violation in total violations.

9.2.1 Pie chart : Dihedral angle violations



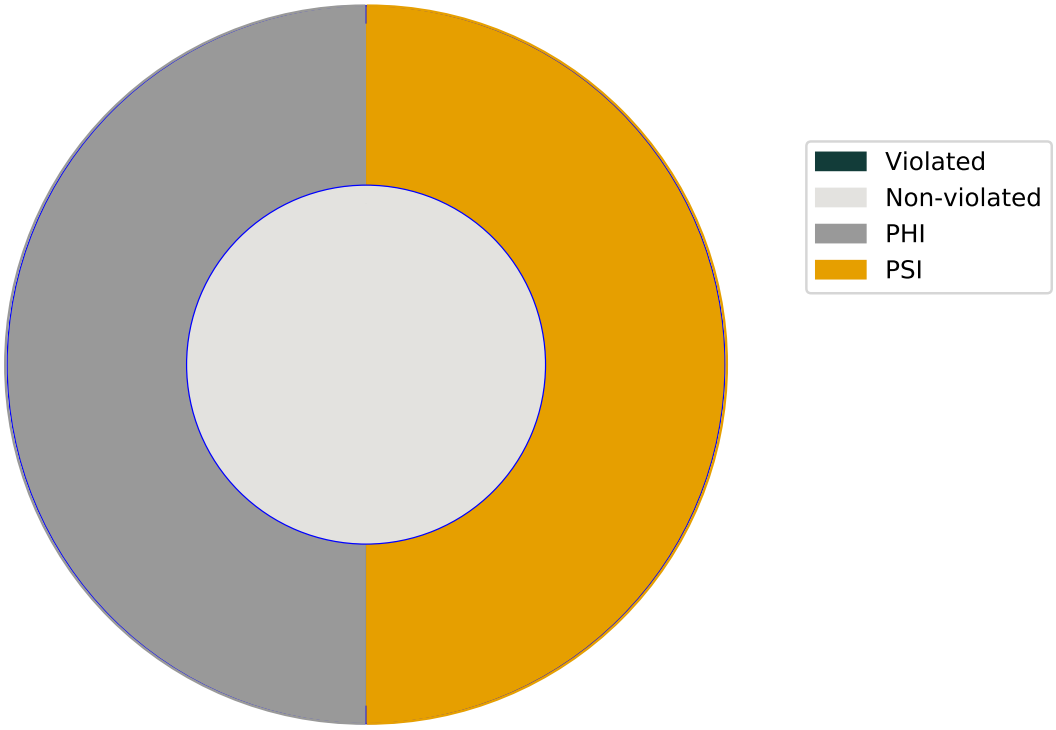
9.3 Consistent dihedral angle violations

The following table provides the summary of consistently violated restraints. Restraints that are violated in all models are counted as consistently violated.

Angle name	Count	%[1]	%[2]
PHI	0	0.0	0.0
PSI	0	0.0	0.0
Total	0	0.0	0.0

[1]percentage of violated restraints in that particular angle type, [2]percentage of violation in total violations.

9.3.1 Pie chart : Consistent dihedral angle violations



9.4 Residual dihedral angle violations

Violation are counted in different bin sizes and listed below

Range (∘)	Avg. No. of violated restraints per model	Max violation (∘)
0.0-5.0	None	None
5.0-10.0	None	None
10.0-20.0	None	None
20.0-40.0	None	None
40.0-80.0	None	None
80.0<	None	None

9.5 Dihedral angle violations in the ensemble

The restraints are grouped based on the number of violated models and listed here.

No. of violated restraints			No. of violated models
PHI	PSI	Total	
0	0	0	1

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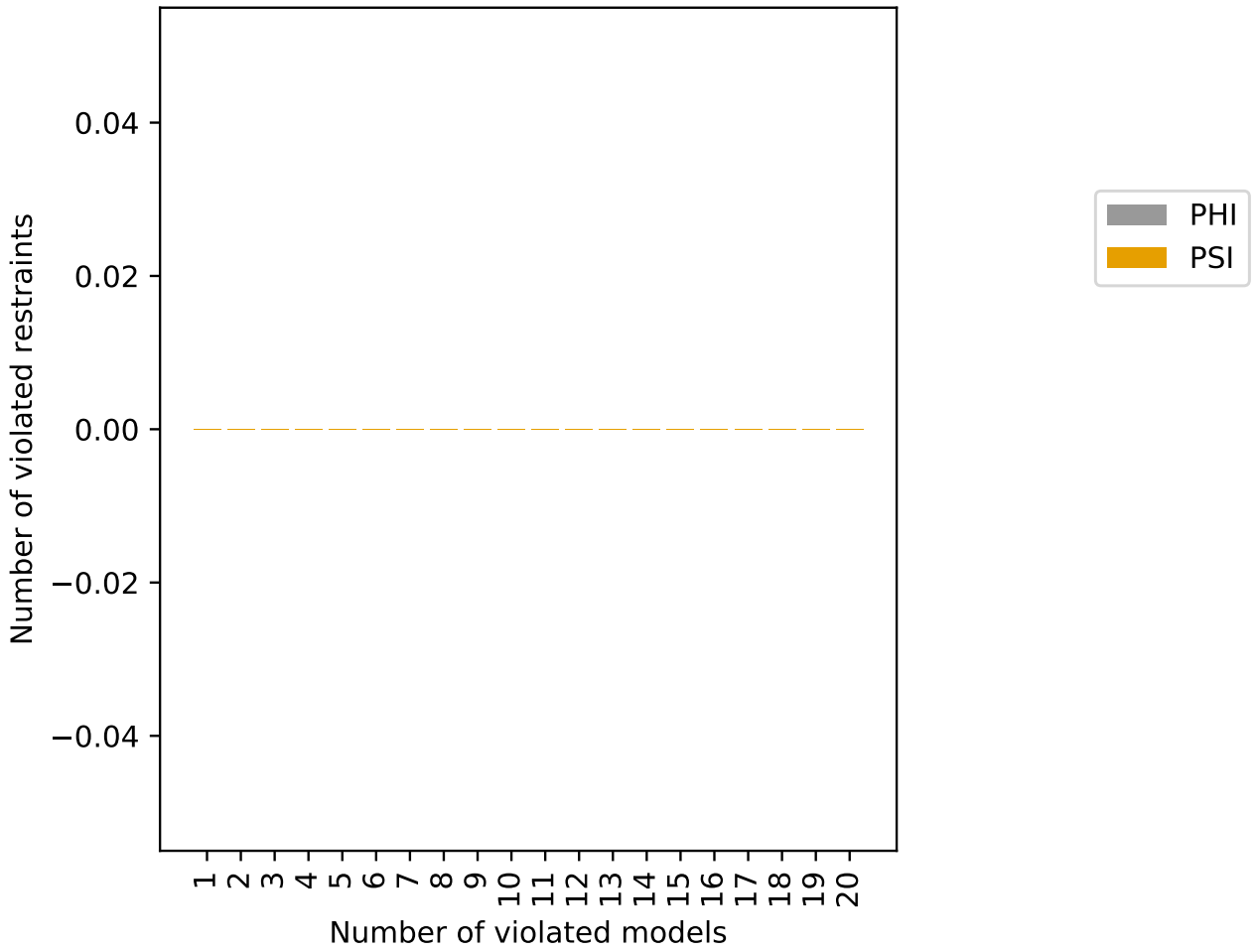
No. of violated restraints			No. of violated models
PHI	PSI	Total	
0	0	0	2
0	0	0	3
0	0	0	4
0	0	0	5
0	0	0	6
0	0	0	7
0	0	0	8
0	0	0	9
0	0	0	10
0	0	0	11
0	0	0	12
0	0	0	13
0	0	0	14
0	0	0	15
0	0	0	16
0	0	0	17
0	0	0	18
0	0	0	19
0	0	0	20

9.5.1 Bar graph : No. of models vs No. of violations



9.6 Violations in each model

The following table lists the violation count in each model in the ensemble

Model ID	No. of violations			Mean (∘)	Max (∘)
	PHI	PSI	Total		
1	0	0	0	0.0	0.0
2	0	0	0	0.0	0.0
3	0	0	0	0.0	0.0
4	0	0	0	0.0	0.0
5	0	0	0	0.0	0.0
6	0	0	0	0.0	0.0
7	0	0	0	0.0	0.0
8	0	0	0	0.0	0.0
9	0	0	0	0.0	0.0

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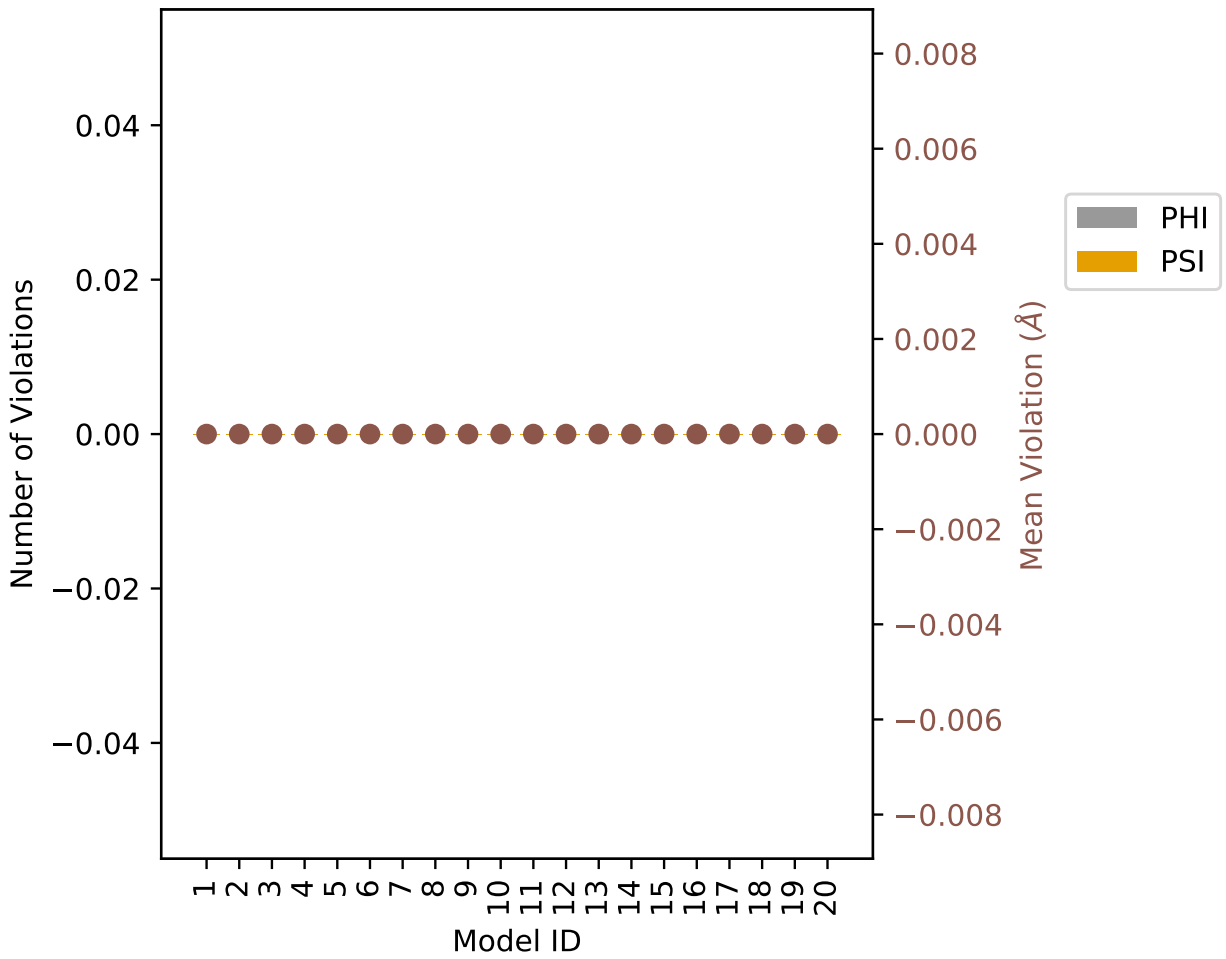
Model ID	No. of violations			Mean (∘)	Max (∘)
	PHI	PSI	Total		
10	0	0	0	0.0	0.0
11	0	0	0	0.0	0.0
12	0	0	0	0.0	0.0
13	0	0	0	0.0	0.0
14	0	0	0	0.0	0.0
15	0	0	0	0.0	0.0
16	0	0	0	0.0	0.0
17	0	0	0	0.0	0.0
18	0	0	0	0.0	0.0
19	0	0	0	0.0	0.0
20	0	0	0	0.0	0.0

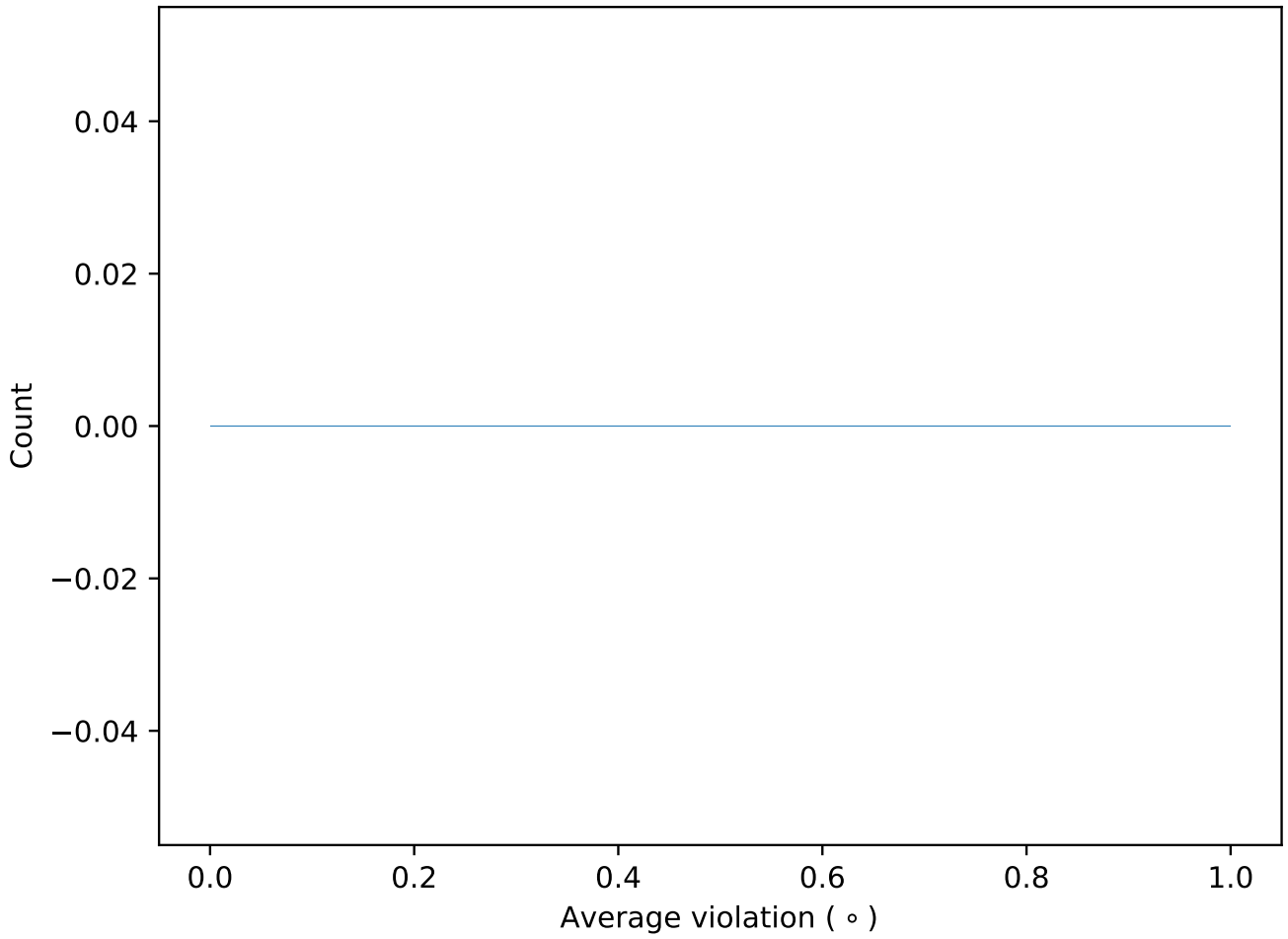
9.6.1 Bar graph : Violations in each model



9.7 Most violated dihedral angle restraints

9.7.1 Histogram : Distribution of mean dihedral angle violations

The following histogram shows the distribution of average violation of each restraint



9.7.2 Table: Most violated dihedral angle restraints

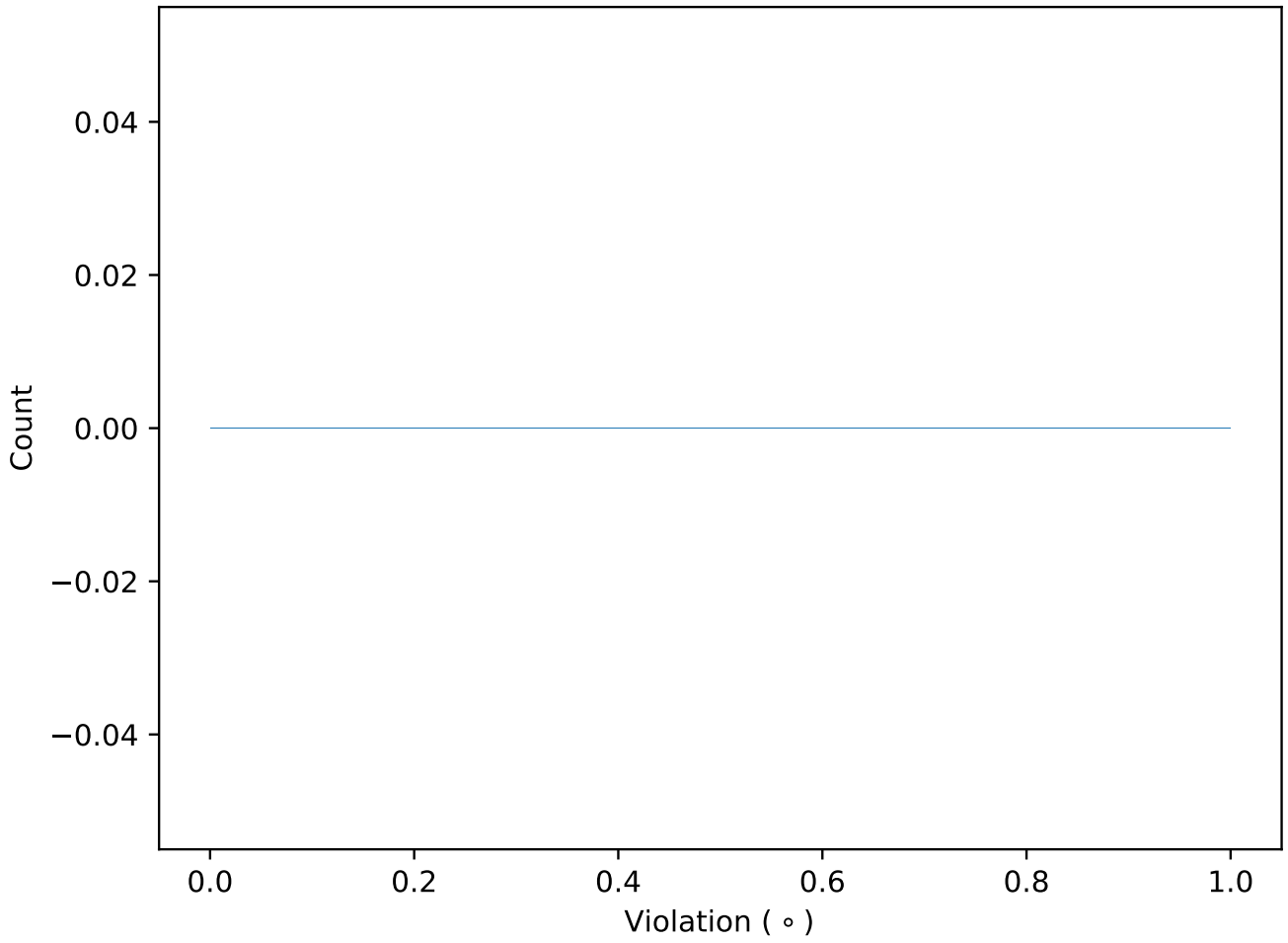
The following tale lists the average violation of each restraint sorted by number of violated models

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (∘)	Max (∘)

9.8 All violated dihedral angleeee restraints

9.8.1 Histogram : Distribution of violations

The following histogram shows the distribution of violations in the ensemble.



9.8.2 Table: All violated dihedral angle restraints

The following table lists the violations in the ensemble sorted by violation value

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)