wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2KO1
Title	:	Solution NMR structure of the ACT domain from GTP pyrophosphokinase of Chlorobium tepidum. Northeast Structural Genomics Consortium Target CtR148A
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Deposited on	:	2009-09-08

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:

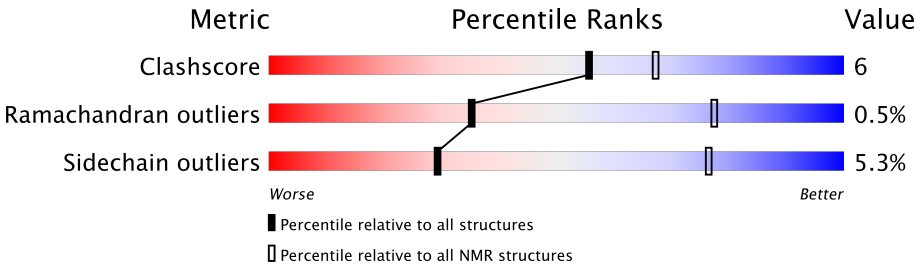
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analalysis	:	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 64%.

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	88	76% 13% 11%
1	B	88	76% 14% 10%

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:4-A:81, B:3-B:81 (157)	0.32	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1452 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1429	442	726	128	128	5	
1	B	88	Total	C	H	N	O	S	0
			1429	442	726	128	128	5	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q8KC80
A	16	ASN	ILE	ENGINEERED	UNP Q8KC80
A	81	LEU	-	EXPRESSION TAG	UNP Q8KC80
A	82	GLU	-	EXPRESSION TAG	UNP Q8KC80
A	83	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	84	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	85	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	86	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	87	HIS	-	EXPRESSION TAG	UNP Q8KC80
A	88	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	1	MET	-	INITIATING METHIONINE	UNP Q8KC80
B	16	ASN	ILE	ENGINEERED	UNP Q8KC80
B	81	LEU	-	EXPRESSION TAG	UNP Q8KC80
B	82	GLU	-	EXPRESSION TAG	UNP Q8KC80
B	83	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	84	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	85	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	86	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	87	HIS	-	EXPRESSION TAG	UNP Q8KC80
B	88	HIS	-	EXPRESSION TAG	UNP Q8KC80

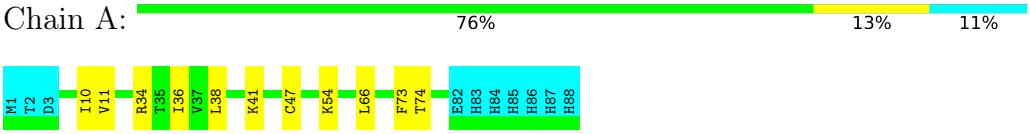
4 Residue-property plots

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.

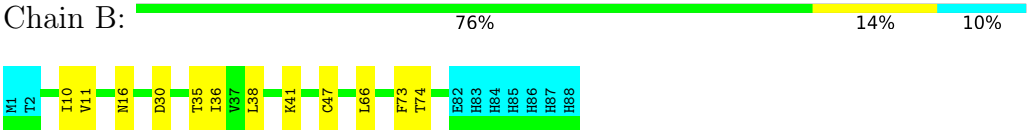
• Molecule 1: GTP pyrophosphokinase

Chain A:



• Molecule 1: GTP pyrophosphokinase

Chain B:

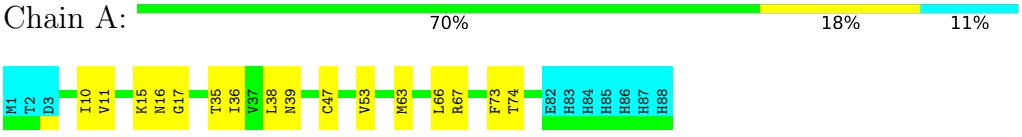


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

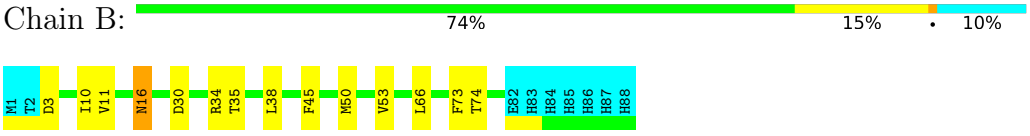
• Molecule 1: GTP pyrophosphokinase

Chain A:



• Molecule 1: GTP pyrophosphokinase

Chain B:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	1.2.1

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)	2ko1_nmr.cif
Number of chemical shift lists	1
Total number of shifts	2170
Number of shifts mapped to atoms	1348
Number of unparsed shifts	312
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	510
Assignment completeness (well-defined parts)	64%

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	610	650	650	8±2
1	B	618	654	654	9±3
All	All	24560	26080	26080	288

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 6.

5 of 104 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:ILE:HD11	1:B:66:LEU:HD13	0.71	1.62	3	11
1:B:36:ILE:HD11	1:B:47:CYS:SG	0.66	2.29	14	10
1:A:10:ILE:HD11	1:A:66:LEU:HD13	0.66	1.65	18	14
1:A:36:ILE:HD11	1:A:47:CYS:SG	0.65	2.31	5	9
1:A:15:LYS:O	1:A:17:GLY:N	0.59	2.35	20	3

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	78/88 (89%)	75±2 (96±3%)	3±2 (4±3%)	0±0 (0±1%)	40 79
1	B	79/88 (90%)	75±2 (95±2%)	4±2 (4±2%)	0±1 (1±1%)	31 76
All	All	3140/3520 (89%)	2996 (95%)	129 (4%)	15 (0%)	35 77

5 of 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	16	ASN	5
1	A	16	ASN	4
1	A	42	ASP	2
1	B	17	GLY	2
1	B	43	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	70/80 (88%)	66±2 (95±2%)	4±2 (5±2%)	29 76
1	B	71/80 (89%)	67±1 (95±2%)	4±1 (5±2%)	30 77
All	All	2820/3200 (88%)	2670 (95%)	150 (5%)	29 76

5 of 41 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	B	73	PHE	19
1	A	41	LYS	17
1	B	41	LYS	13
1	A	73	PHE	13
1	B	30	ASP	11

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: 2ko1_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_aco.tbl*

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	2170
Number of shifts mapped to atoms	1348
Number of unparsed shifts	312
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	510
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 312) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
4	A	2	THR	HG2%	1.335	0.020	1
5	A	2	THR	HG2%	1.335	0.020	1
21	A	4	PHE	HB%	3.080	0.020	1
23	A	4	PHE	HD%	7.184	0.020	1
38	A	5	LEU	HD1%	0.475	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 510) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	21	GLN	HBx	2.243	0.02	2
B	44	ILE	HG1x	1.482	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	LEU	HBx	1.26	0.02	2
B	41	LYS	HB%	1.815	0.02	1
A	33	ILE	HG1x	1.751	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
$^{13}C_{\alpha}$	164	-0.11 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	152	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	162	0.07 ± 0.13	None needed (< 0.5 ppm)
^{15}N	162	-0.06 ± 0.17	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 64%, i.e. 1256 atoms were assigned a chemical shift out of a possible 1959. 30 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	771/785 (98%)	302/314 (96%)	312/314 (99%)	157/157 (100%)
Sidechain	445/1084 (41%)	72/622 (12%)	347/406 (85%)	26/56 (46%)
Aromatic	40/90 (44%)	20/50 (40%)	20/40 (50%)	0/0 (—%)
Overall	1256/1959 (64%)	394/986 (40%)	679/760 (89%)	183/213 (86%)

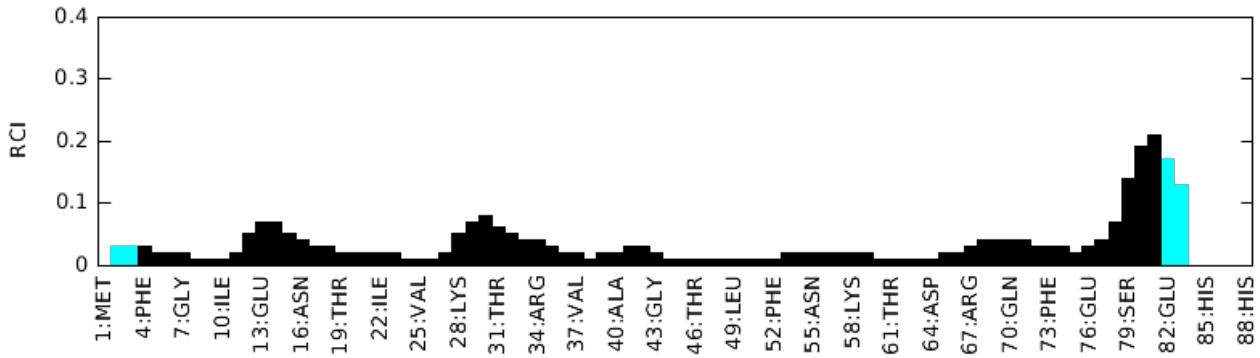
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

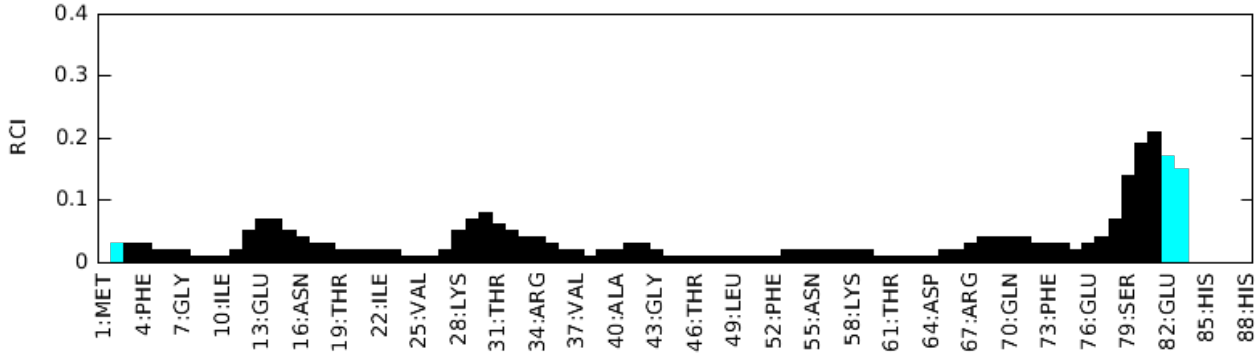
7.1.5 Random Coil Index (RCI) plots (i)

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 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	5014
Intra-residue (|i-j|=0)	827
Sequential (|i-j|=1)	1154
Medium range (|i-j|>1 and |i-j|<5)	1035
Long range (|i-j|≥5)	1862
Inter-chain	136
Total dihedral-anlge restraints	232
Total hydrogen bond restraints	0
Total disulfide bond restraints	0
Number of unmapped restraints	0
Number of restraints per residue	3.4
Number of long range restraints per residue	1.3

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.7	0.2
0.2-0.5 (Medium)	2.3	0.39
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-anlge violations per model

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	10.5	3.6
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

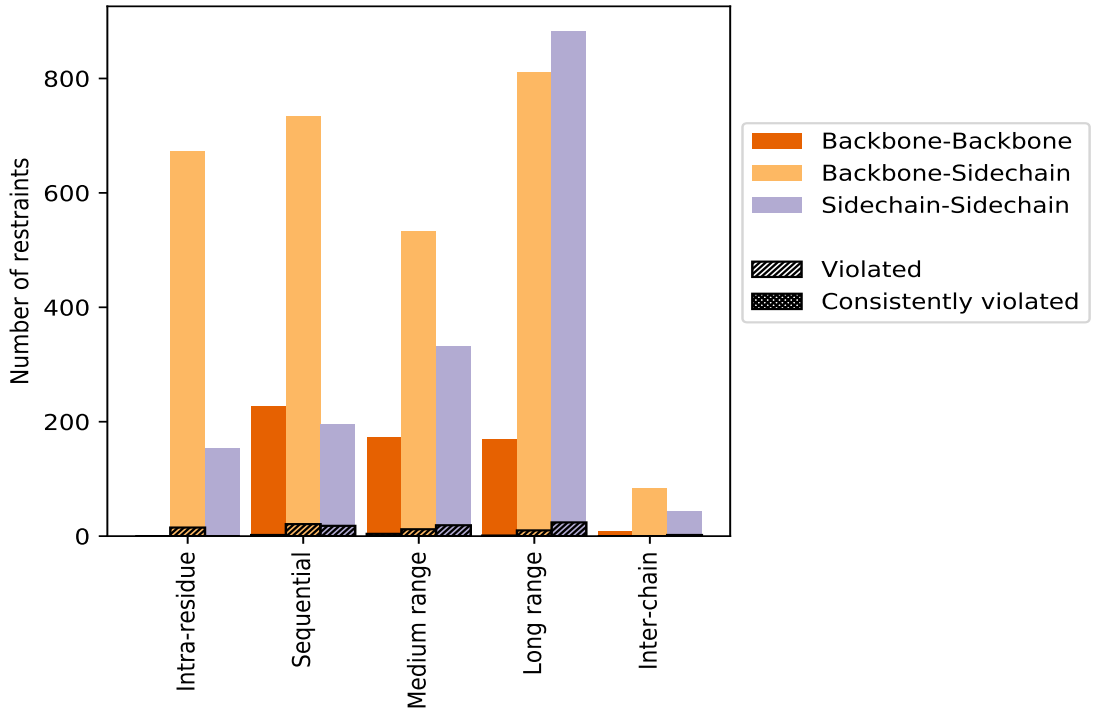
9.1 Summary of distance violations

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	827	16.5	15	1.8	0.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	673	13.4	15	2.2	0.3	0	0.0	0.0
Sidechain-Sidechain	154	3.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1154	23.0	41	3.6	0.8	0	0.0	0.0
Backbone-Backbone	226	4.5	2	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	733	14.6	21	2.9	0.4	0	0.0	0.0
Sidechain-Sidechain	195	3.9	18	9.2	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1035	20.6	35	3.4	0.7	0	0.0	0.0
Backbone-Backbone	172	3.4	4	2.3	0.1	0	0.0	0.0
Backbone-Sidechain	532	10.6	12	2.3	0.2	0	0.0	0.0
Sidechain-Sidechain	331	6.6	19	5.7	0.4	0	0.0	0.0
Long range (|i-j|≥5)	1862	37.1	35	1.9	0.7	0	0.0	0.0
Backbone-Backbone	170	3.4	1	0.6	0.0	0	0.0	0.0
Backbone-Sidechain	810	16.2	10	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	882	17.6	24	2.7	0.5	0	0.0	0.0
Inter-chain	136	2.7	2	1.5	0.0	0	0.0	0.0
Backbone-Backbone	8	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	84	1.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	44	0.9	2	4.5	0.0	0	0.0	0.0
Total	5014	100.0	128	2.6	2.6	0	0.0	0.0
Backbone-Backbone	576	11.5	7	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	2832	56.5	58	2.0	1.2	0	0.0	0.0
Sidechain-Sidechain	1606	32.0	63	3.9	1.3	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total			
1	3	11	7	3	0	24	0.17	0.39	0.08
2	1	6	9	4	0	20	0.15	0.36	0.06
3	1	6	6	2	0	15	0.16	0.32	0.06
4	3	4	5	8	0	20	0.14	0.21	0.03
5	2	5	6	5	0	18	0.14	0.36	0.06
6	2	3	3	2	0	10	0.15	0.21	0.04
7	3	8	4	6	0	21	0.15	0.25	0.04
8	2	6	4	4	0	16	0.15	0.29	0.06
9	0	4	6	2	0	12	0.13	0.16	0.02
10	3	4	8	5	1	21	0.14	0.3	0.05
11	2	3	3	4	0	12	0.14	0.24	0.04
12	5	3	7	6	0	21	0.14	0.24	0.03

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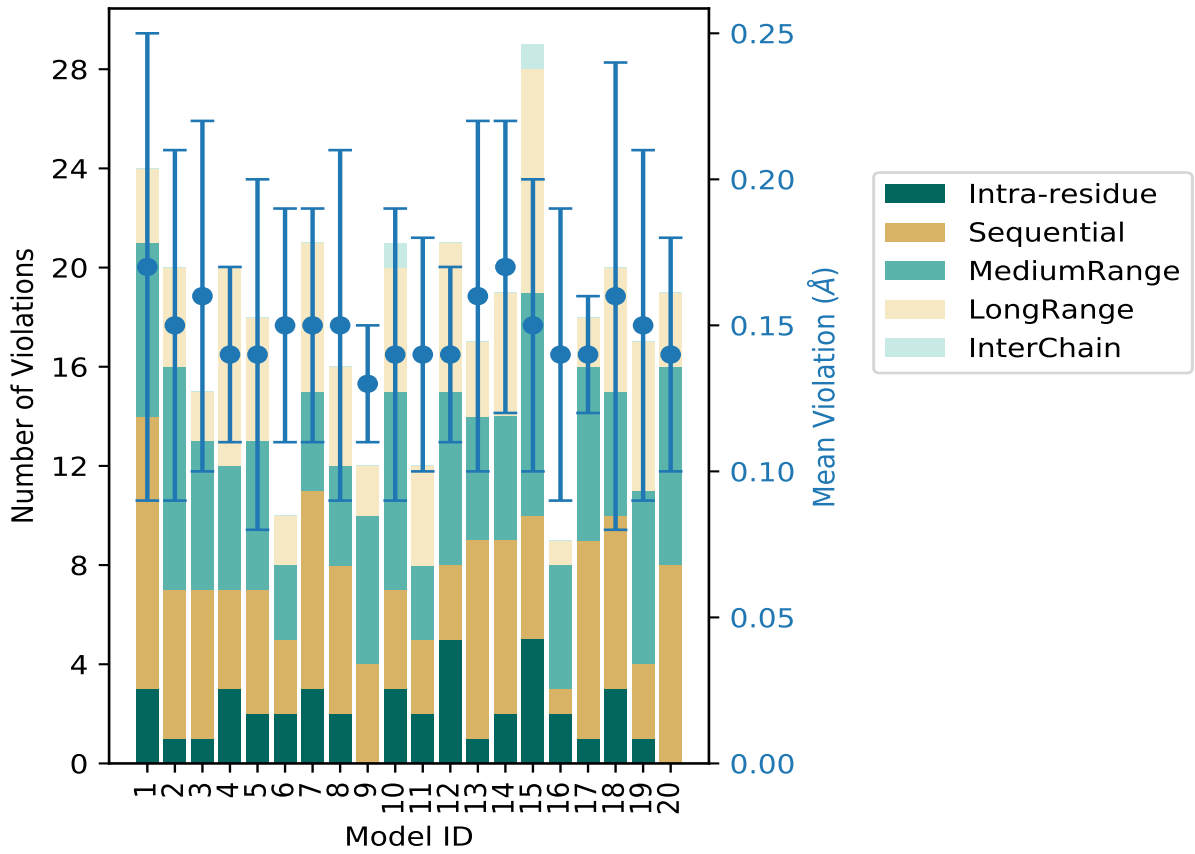
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total			
13	1	8	5	3	0	17	0.16	0.37	0.06
14	2	7	5	5	0	19	0.17	0.28	0.05
15	5	5	9	9	1	29	0.15	0.33	0.05
16	2	1	5	1	0	9	0.14	0.27	0.05
17	1	8	7	2	0	18	0.14	0.18	0.02
18	3	7	5	5	0	20	0.16	0.34	0.08
19	1	3	7	6	0	17	0.15	0.33	0.06
20	0	8	8	3	0	19	0.14	0.29	0.04

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

9.2.1 Bar graph : Distance Violation statistics for each model



The mean and the standard deviation are shown in blue with respect to the y axis on the right

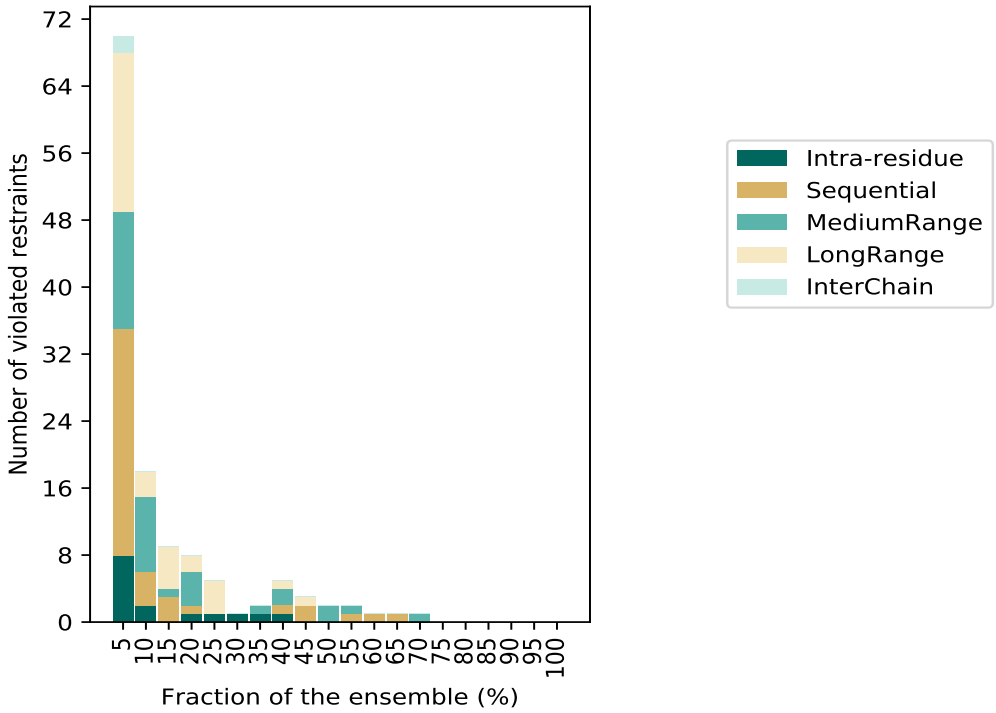
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4886(IR:812, SQ:1113, MR:1000, LR:1827, IC:134) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
8	27	14	19	2	70	1	5.0
2	4	9	3	0	18	2	10.0
0	3	1	5	0	9	3	15.0
1	1	4	2	0	8	4	20.0
1	0	0	4	0	5	5	25.0
1	0	0	0	0	1	6	30.0
1	0	1	0	0	2	7	35.0
1	1	2	1	0	5	8	40.0
0	2	0	1	0	3	9	45.0
0	0	2	0	0	2	10	50.0
0	1	1	0	0	2	11	55.0
0	1	0	0	0	1	12	60.0
0	1	0	0	0	1	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

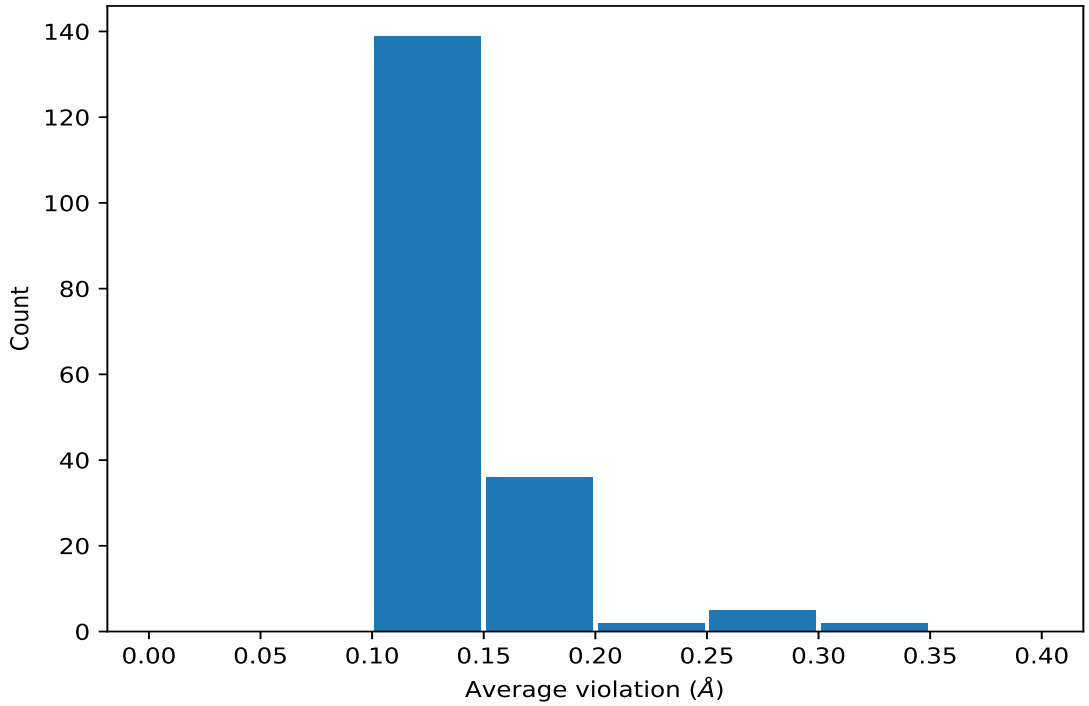
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	14	0.13	0.02
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	13	0.18	0.05
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	13	0.18	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	13	0.18	0.05
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	13	0.18	0.05
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	12	0.15	0.04
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	12	0.15	0.04
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	12	0.15	0.04
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	11	0.19	0.06
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	11	0.19	0.06
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	11	0.19	0.06
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	11	0.19	0.06
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	11	0.13	0.02
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	10	0.12	0.01
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	10	0.12	0.01
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	10	0.12	0.01

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	10	0.13	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	9	0.12	0.01
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	9	0.12	0.01
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	9	0.14	0.02
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	9	0.14	0.02
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	9	0.14	0.02
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	9	0.15	0.02
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	9	0.15	0.02
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	9	0.15	0.02
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	8	0.13	0.02
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	8	0.13	0.02
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	8	0.13	0.02
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	8	0.25	0.07
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	8	0.25	0.07
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	8	0.16	0.02
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	8	0.16	0.02
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	8	0.16	0.02
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	8	0.15	0.03
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	8	0.15	0.03
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	8	0.15	0.03
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	8	0.12	0.01
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	7	0.17	0.05
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	7	0.22	0.06
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	7	0.22	0.06
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	6	0.14	0.02
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	5	0.11	0.0
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	5	0.11	0.0
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	5	0.11	0.0
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	5	0.12	0.01
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	5	0.12	0.01
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	5	0.12	0.01
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	5	0.25	0.09
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	5	0.25	0.09
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	5	0.11	0.0
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	5	0.11	0.0

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	5	0.11	0.0
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	5	0.12	0.01
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	5	0.12	0.01
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	5	0.12	0.01
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	4	0.15	0.03
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	4	0.15	0.03
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	4	0.13	0.02
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	4	0.13	0.02
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	4	0.13	0.02
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	4	0.13	0.02
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	4	0.13	0.02
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	4	0.13	0.02
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	4	0.25	0.08
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	4	0.19	0.1
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	4	0.13	0.01
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	4	0.13	0.01
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	4	0.13	0.01
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	4	0.14	0.02
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	4	0.14	0.02
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	4	0.16	0.03
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	4	0.13	0.02
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	4	0.13	0.02
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	3	0.32	0.03
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	3	0.32	0.03
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	3	0.17	0.06
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	3	0.17	0.06
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	3	0.17	0.06
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	3	0.17	0.06

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	3	0.17	0.06
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	3	0.17	0.06
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	3	0.15	0.02
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	3	0.15	0.02
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	3	0.15	0.02
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	3	0.15	0.02
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	3	0.15	0.02
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	3	0.15	0.02
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	3	0.13	0.01
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	3	0.13	0.01
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	3	0.13	0.01
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	3	0.16	0.04
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	3	0.16	0.04
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	3	0.16	0.02
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	3	0.16	0.02
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	3	0.16	0.02
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	3	0.12	0.01
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	3	0.12	0.01
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	3	0.12	0.01
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	3	0.14	0.02
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	3	0.14	0.02
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	3	0.14	0.02
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	3	0.14	0.02
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	3	0.14	0.02
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	3	0.14	0.02
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	3	0.11	0.0
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	3	0.11	0.0
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	3	0.11	0.0
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	2	0.14	0.03
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	2	0.14	0.03
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	2	0.14	0.03
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	2	0.14	0.03
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	2	0.11	0.0
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	2	0.11	0.0
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	2	0.11	0.0
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	2	0.11	0.0
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	2	0.11	0.0
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	2	0.11	0.0
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	2	0.13	0.01
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	2	0.13	0.01
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	2	0.13	0.01
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	2	0.13	0.01

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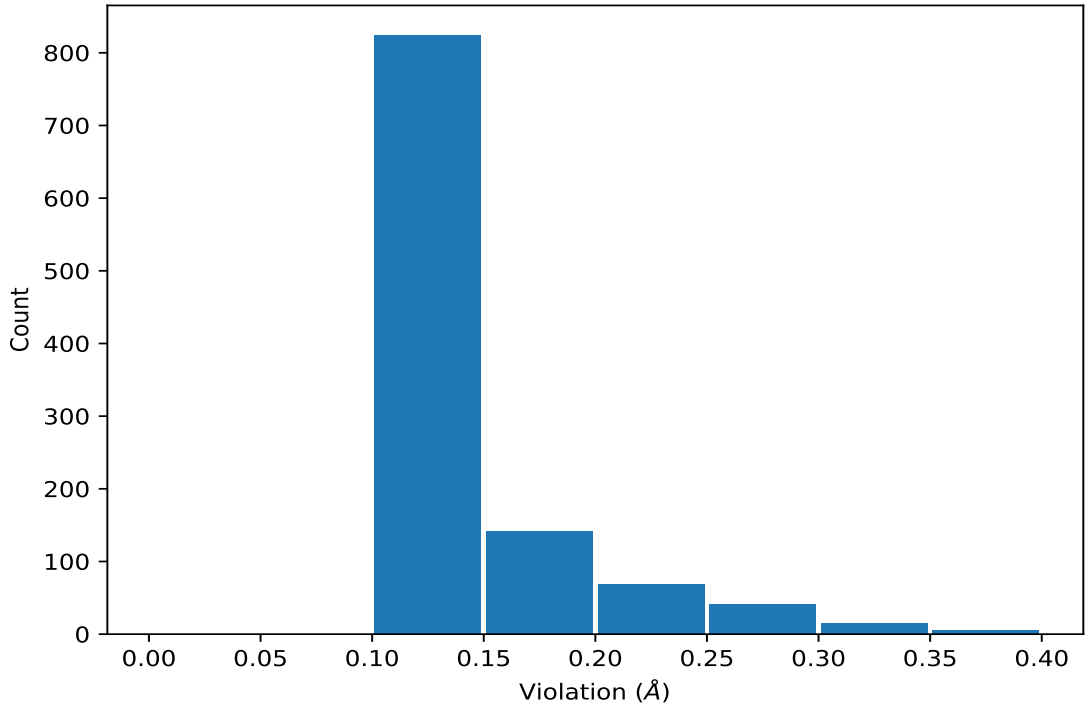
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	2	0.13	0.01
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	2	0.13	0.01
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	2	0.13	0.01
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	2	0.13	0.01
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	2	0.13	0.01
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	2	0.12	0.01
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	2	0.12	0.01
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	2	0.12	0.01
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	2	0.12	0.01
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	2	0.12	0.01
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	2	0.14	0.01
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	2	0.11	0.0
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	2	0.11	0.0
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	2	0.11	0.0
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	2	0.19	0.06
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	2	0.19	0.06
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	2	0.13	0.01
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	2	0.13	0.01
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	2	0.15	0.04
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	2	0.15	0.04
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	2	0.19	0.03
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	2	0.19	0.03
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	2	0.19	0.03
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	2	0.19	0.03
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	2	0.19	0.03
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	2	0.19	0.03
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	2	0.19	0.03
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	2	0.19	0.03
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	2	0.19	0.03
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	2	0.13	0.02
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	2	0.13	0.02
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	2	0.14	0.02
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	2	0.14	0.02
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	2	0.14	0.02
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	2	0.11	0.0
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	2	0.11	0.0
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	2	0.11	0.0
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	2	0.12	0.01
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	2	0.13	0.02
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	2	0.12	0.01
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	2	0.12	0.01
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	2	0.12	0.01

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

9.5 All distance violations

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4050)	1:A:41:LYS:HA	1:A:42:ASP:H	1	0.39
(1,4051)	1:B:41:LYS:HA	1:B:42:ASP:H	13	0.37
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	2	0.36
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	2	0.36
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	5	0.36
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	18	0.34
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	18	0.33
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	18	0.33
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	18	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	1	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	1	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	19	0.33
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	19	0.33
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	15	0.33
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	15	0.33
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	3	0.32
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	3	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	3	0.32
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	3	0.32
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	10	0.3
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	10	0.3
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	20	0.29
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	8	0.29
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	8	0.29
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG2	14	0.28
(1,4715)	1:A:81:LEU:H	1:A:82:GLU:HG3	14	0.28
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	14	0.28
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	14	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	14	0.28
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	14	0.28
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	8	0.28
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	8	0.28
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	1	0.27
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	16	0.27
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	16	0.27
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	1	0.27
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	1	0.27
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	1	0.26
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	1	0.26
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	1	0.26
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	1	0.26
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	8	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	15	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	15	0.26
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	15	0.26
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	3	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	3	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	10	0.26
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	10	0.26
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG2	7	0.25
(1,5014)	1:B:81:LEU:H	1:B:82:GLU:HG3	7	0.25
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	15	0.25
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	15	0.25
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	15	0.25
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	15	0.25
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	7	0.25
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	7	0.25
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	11	0.24
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	11	0.24
(1,2162)	1:B:28:LYS:HA	1:B:28:LYS:HG2	12	0.24
(1,176)	1:B:15:LYS:H	1:B:18:MET:HG2	14	0.24
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	7	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	7	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	7	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	7	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	15	0.23
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	15	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	15	0.23
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	15	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	18	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	18	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	18	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	18	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	19	0.23
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	19	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	19	0.23
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	19	0.23
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	2	0.23
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	2	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE2	3	0.23
(1,3397)	1:B:60:THR:HG21	1:B:63:MET:HE3	3	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE2	3	0.23
(1,3397)	1:B:60:THR:HG22	1:B:63:MET:HE3	3	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE1	3	0.23
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3397)	1:B:60:THR:HG23	1:B:63:MET:HE3	3	0.23
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	1	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	14	0.22
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	14	0.22
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	13	0.21
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	5	0.21
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	5	0.21
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	19	0.21
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	19	0.21
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	6	0.21
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	13	0.21
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	13	0.21
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	13	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	4	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	4	0.21
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	4	0.21
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	4	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	4	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	4	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	4	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	14	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	14	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	14	0.2
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	14	0.2
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	1	0.2
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	1	0.2
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	3	0.2
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	3	0.2
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	3	0.2
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	1	0.19
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	1	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	1	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	11	0.19
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	11	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	11	0.19
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	11	0.19
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	6	0.19
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	6	0.19
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	2	0.19
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	2	0.19
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	13	0.19
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	8	0.19
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	8	0.19
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	8	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	10	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	10	0.19
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	10	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	12	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	12	0.19
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	12	0.19
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	4	0.18
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	4	0.18
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	17	0.18
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	17	0.18
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD1	12	0.18
(1,4719)	1:B:3:ASP:HB2	1:B:52:PHE:HD2	12	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD1	12	0.18
(1,4719)	1:B:3:ASP:HB3	1:B:52:PHE:HD2	12	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	14	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	14	0.18
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	14	0.18
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	14	0.18
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	7	0.18
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	14	0.18
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	14	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	6	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	8	0.18
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	8	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	3	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	15	0.18
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	15	0.18
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	11	0.17
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	11	0.17
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	11	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	7	0.17
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	7	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	6	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	6	0.17
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	6	0.17
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	19	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	7	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	7	0.17
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	7	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	17	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	17	0.17
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	17	0.17
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	17	0.17
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	7	0.16
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	7	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	7	0.16
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	7	0.16
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	16	0.16
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	16	0.16
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	16	0.16
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	16	0.16
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	20	0.16
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	20	0.16
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	20	0.16
(1,4405)	1:A:3:ASP:HB2	1:A:4:PHE:H	17	0.16
(1,4405)	1:A:3:ASP:HB3	1:A:4:PHE:H	17	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG21	1:A:63:MET:HE3	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG22	1:A:63:MET:HE3	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE1	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE2	2	0.16
(1,3396)	1:A:60:THR:HG23	1:A:63:MET:HE3	2	0.16
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE2	12	0.16
(1,3106)	1:B:54:LYS:H	1:B:54:LYS:HE3	12	0.16
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	12	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	5	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	5	0.16
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	5	0.16
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	9	0.16
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	9	0.16
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	9	0.16
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	7	0.16
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	7	0.16
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	7	0.16
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	9	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	1	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	18	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	18	0.16
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	18	0.16
(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE2	12	0.16
(1,2178)	1:B:28:LYS:HA	1:B:28:LYS:HE3	12	0.16
(1,2167)	1:A:27:SER:HG	1:A:28:LYS:HG3	20	0.16
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG21	1	0.16
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG22	1	0.16
(1,1814)	1:A:68:LYS:HE2	1:A:69:VAL:HG23	1	0.16
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG21	1	0.16
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG22	1	0.16
(1,1814)	1:A:68:LYS:HE3	1:A:69:VAL:HG23	1	0.16
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	4	0.16
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	4	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	4	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	4	0.16
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	4	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	4	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	4	0.16
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	4	0.16
(1,1021)	1:B:58:LYS:HZ1	1:B:61:THR:H	4	0.16
(1,1021)	1:B:58:LYS:HZ2	1:B:61:THR:H	4	0.16
(1,1021)	1:B:58:LYS:HZ3	1:B:61:THR:H	4	0.16
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG21	19	0.15
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG22	19	0.15
(1,4745)	1:B:9:ARG:HG2	1:B:11:VAL:HG23	19	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG21	19	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG22	19	0.15
(1,4745)	1:B:9:ARG:HG3	1:B:11:VAL:HG23	19	0.15
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	1	0.15
(1,4643)	1:A:54:LYS:HE2	1:A:55:ASN:HD22	1	0.15
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	1	0.15
(1,4643)	1:A:54:LYS:HE3	1:A:55:ASN:HD22	1	0.15
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	10	0.15
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	10	0.15
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	10	0.15
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	10	0.15
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	10	0.15
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	10	0.15
(1,4397)	1:B:82:GLU:HA	1:B:83:HIS:HD2	5	0.15
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	17	0.15
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	2	0.15
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	19	0.15
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	19	0.15
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	19	0.15
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	19	0.15
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	19	0.15
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	19	0.15
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	20	0.15
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	20	0.15
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	15	0.15
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	15	0.15
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	10	0.15
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	10	0.15
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	10	0.15
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	14	0.15
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	10	0.15
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	10	0.15
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	10	0.15
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	18	0.15
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	18	0.15
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	18	0.15
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	4	0.15
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	11	0.15
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	11	0.15
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	11	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	2	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	3	0.15
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	17	0.15
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	17	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	3	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	3	0.15
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	3	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	14	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	14	0.15
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	14	0.15
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	14	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG21	15	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG22	15	0.15
(1,2106)	1:B:21:GLN:HE22	1:B:25:VAL:HG23	15	0.15
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD2	13	0.15
(1,1378)	1:B:40:ALA:H	1:B:41:LYS:HD3	13	0.15
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	2	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	2	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	2	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	17	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	17	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	17	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	17	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	18	0.14
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	18	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	18	0.14
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	18	0.14
(1,4647)	1:A:55:ASN:HD21	1:A:57:ASP:HB2	15	0.14
(1,4647)	1:A:55:ASN:HD21	1:A:57:ASP:HB3	15	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB2	15	0.14
(1,4647)	1:A:55:ASN:HD22	1:A:57:ASP:HB3	15	0.14
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	2	0.14
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	2	0.14
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	2	0.14
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	2	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	9	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	9	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	9	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	9	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	10	0.14
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	10	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	10	0.14
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	10	0.14
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	6	0.14
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	14	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	14	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	16	0.14
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	17	0.14
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	17	0.14
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	17	0.14
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	10	0.14
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	10	0.14
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	10	0.14
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	9	0.14
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	12	0.14
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	12	0.14
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE2	15	0.14
(1,3480)	1:B:65:LYS:HA	1:B:65:LYS:HE3	15	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	2	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	2	0.14
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	2	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	1	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	12	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	12	0.14
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	12	0.14
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD2	4	0.14
(1,3100)	1:B:54:LYS:H	1:B:54:LYS:HD3	4	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	13	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	13	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	14	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	14	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	19	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	19	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	19	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	19	0.14
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:A:33:ILE:HG13	1:B:20:ASN:HD22	15	0.14
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	11	0.14
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	16	0.14
(1,2679)	1:A:9:ARG:HG2	1:A:48:ASN:HA	9	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG21	19	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG22	19	0.14
(1,2630)	1:B:9:ARG:HE	1:B:46:THR:HG23	19	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	3	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	13	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	17	0.14
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	18	0.14
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	18	0.14
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	18	0.14
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	20	0.14
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	5	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	7	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	7	0.14
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	7	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	2	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	12	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	12	0.14
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	12	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD11	8	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD12	8	0.14
(1,231)	1:B:19:THR:H	1:B:38:LEU:HD13	8	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	13	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	13	0.14
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	13	0.14
(1,2174)	1:B:68:LYS:HA	1:B:68:LYS:HD2	15	0.14
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	9	0.14
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	18	0.14
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	14	0.14
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG21	1:B:41:LYS:HE3	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG22	1:B:41:LYS:HE3	15	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE2	15	0.14
(1,1809)	1:B:11:VAL:HG23	1:B:41:LYS:HE3	15	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG11	4	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG12	4	0.14
(1,1760)	1:A:13:GLU:HG2	1:A:69:VAL:HG13	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG11	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG12	4	0.14
(1,1760)	1:A:13:GLU:HG3	1:A:69:VAL:HG13	4	0.14
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	2	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	19	0.14
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	19	0.14
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD2	1	0.14
(1,1377)	1:A:40:ALA:H	1:A:41:LYS:HD3	1	0.14
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	20	0.13
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	20	0.13
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	12	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	12	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	12	0.13
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	12	0.13
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	12	0.13
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	12	0.13
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	12	0.13
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	12	0.13
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	17	0.13
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	17	0.13
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	17	0.13
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	2	0.13
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	2	0.13
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	2	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	4	0.13
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	4	0.13
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	14	0.13
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	14	0.13
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	18	0.13
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	10	0.13
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	10	0.13
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	10	0.13
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	5	0.13
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	5	0.13
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	5	0.13
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG2	13	0.13
(1,3622)	1:B:69:VAL:HA	1:B:70:GLN:HG3	13	0.13
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG2	7	0.13
(1,3621)	1:A:69:VAL:HA	1:A:70:GLN:HG3	7	0.13
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG11	1:B:70:GLN:HB3	14	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG12	1:B:70:GLN:HB3	14	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB2	14	0.13
(1,3606)	1:B:69:VAL:HG13	1:B:70:GLN:HB3	14	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	17	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	17	0.13
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	17	0.13
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	17	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG11	20	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG12	20	0.13
(1,3569)	1:A:15:LYS:HD2	1:A:69:VAL:HG13	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG11	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG12	20	0.13
(1,3569)	1:A:15:LYS:HD3	1:A:69:VAL:HG13	20	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	10	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	10	0.13
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	10	0.13
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	18	0.13
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	18	0.13
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	18	0.13
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	18	0.13
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	18	0.13
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	18	0.13
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	18	0.13
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	18	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	2	0.13
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	2	0.13
(1,277)	1:A:20:ASN:H	1:A:20:ASN:HD22	7	0.13
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	20	0.13
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	20	0.13
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	20	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	5	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	7	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	9	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	11	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	12	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	13	0.13
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	15	0.13
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	4	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD11	20	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD12	20	0.13
(1,2312)	1:B:35:THR:HB	1:B:36:ILE:HD13	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	10	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	20	0.13
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	20	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	7	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	7	0.13
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	7	0.13
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	15	0.13
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	15	0.13
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	15	0.13
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	10	0.13
(1,2017)	1:A:22:ILE:HD11	1:A:23:THR:HA	17	0.13
(1,2017)	1:A:22:ILE:HD12	1:A:23:THR:HA	17	0.13
(1,2017)	1:A:22:ILE:HD13	1:A:23:THR:HA	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	13	0.13
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	16	0.13
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	19	0.13
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	8	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	1	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	1	0.13
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	1	0.13
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	1	0.13
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	5	0.13
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	5	0.13
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	5	0.13
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG21	1:A:77:ARG:HD3	13	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG22	1:A:77:ARG:HD3	13	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD2	13	0.13
(1,1519)	1:A:8:ILE:HG23	1:A:77:ARG:HD3	13	0.13
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	3	0.13
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	3	0.13
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	3	0.13
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG21	10	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG22	10	0.12
(1,82)	1:A:9:ARG:HE	1:A:11:VAL:HG23	10	0.12
(1,727)	1:B:41:LYS:HB2	1:B:42:ASP:H	13	0.12
(1,727)	1:B:41:LYS:HB3	1:B:42:ASP:H	13	0.12
(1,563)	1:A:32:ASN:HD21	1:A:33:ILE:HB	15	0.12
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG11	1:B:70:GLN:HE22	17	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG12	1:B:70:GLN:HE22	17	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE21	17	0.12
(1,5002)	1:B:69:VAL:HG13	1:B:70:GLN:HE22	17	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE1	8	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE2	8	0.12
(1,4916)	1:B:48:ASN:HD21	1:B:50:MET:HE3	8	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE1	8	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE2	8	0.12
(1,4916)	1:B:48:ASN:HD22	1:B:50:MET:HE3	8	0.12
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG21	1:B:58:LYS:HE3	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG22	1:B:58:LYS:HE3	20	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE2	20	0.12
(1,4851)	1:B:31:THR:HG23	1:B:58:LYS:HE3	20	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	5	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	5	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	5	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	5	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB2	13	0.12
(1,4767)	1:B:15:LYS:HG2	1:B:16:ASN:HB3	13	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB2	13	0.12
(1,4767)	1:B:15:LYS:HG3	1:B:16:ASN:HB3	13	0.12
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	11	0.12
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	11	0.12
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	11	0.12
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	11	0.12
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG21	1:A:58:LYS:HE3	14	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG22	1:A:58:LYS:HE3	14	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE2	14	0.12
(1,4560)	1:A:31:THR:HG23	1:A:58:LYS:HE3	14	0.12
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD2	2	0.12
(1,4538)	1:A:27:SER:HG	1:A:28:LYS:HD3	2	0.12
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG21	1:A:28:LYS:HG3	16	0.12
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG22	1:A:28:LYS:HG3	16	0.12
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG2	16	0.12
(1,4524)	1:A:25:VAL:HG23	1:A:28:LYS:HG3	16	0.12
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	5	0.12
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	5	0.12
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	5	0.12
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	5	0.12
(1,4401)	1:B:81:LEU:HD11	1:B:83:HIS:HE1	15	0.12
(1,4401)	1:B:81:LEU:HD12	1:B:83:HIS:HE1	15	0.12
(1,4401)	1:B:81:LEU:HD13	1:B:83:HIS:HE1	15	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	1	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	1	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	11	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	11	0.12
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	11	0.12
(1,4127)	1:B:83:HIS:HA	1:B:83:HIS:HB3	5	0.12
(1,4073)	1:B:60:THR:HB	1:B:61:THR:H	3	0.12
(1,3995)	1:B:82:GLU:H	1:B:83:HIS:HB3	20	0.12
(1,3994)	1:A:82:GLU:H	1:A:83:HIS:HB3	17	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	6	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	6	0.12
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	6	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	7	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	9	0.12
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	18	0.12
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	18	0.12
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	18	0.12
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	12	0.12
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	20	0.12
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	20	0.12
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	20	0.12
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB2	11	0.12
(1,3613)	1:A:69:VAL:H	1:A:70:GLN:HB3	11	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG11	4	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG12	4	0.12
(1,3570)	1:B:15:LYS:HD2	1:B:69:VAL:HG13	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG11	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG12	4	0.12
(1,3570)	1:B:15:LYS:HD3	1:B:69:VAL:HG13	4	0.12
(1,3560)	1:B:15:LYS:HE2	1:B:16:ASN:HD21	6	0.12
(1,3560)	1:B:15:LYS:HE3	1:B:16:ASN:HD21	6	0.12
(1,3559)	1:A:15:LYS:HE2	1:A:16:ASN:HD21	7	0.12
(1,3559)	1:A:15:LYS:HE3	1:A:16:ASN:HD21	7	0.12
(1,3484)	1:B:41:LYS:HE2	1:B:44:ILE:H	9	0.12
(1,3484)	1:B:41:LYS:HE3	1:B:44:ILE:H	9	0.12
(1,3410)	1:A:63:MET:HE1	1:A:77:ARG:HA	4	0.12
(1,3410)	1:A:63:MET:HE2	1:A:77:ARG:HA	4	0.12
(1,3410)	1:A:63:MET:HE3	1:A:77:ARG:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	15	0.12
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	15	0.12
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	15	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG21	2	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG22	2	0.12
(1,3129)	1:A:4:PHE:HD1	1:A:56:THR:HG23	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG21	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG22	2	0.12
(1,3129)	1:A:4:PHE:HD2	1:A:56:THR:HG23	2	0.12
(1,3098)	1:B:15:LYS:HD2	1:B:16:ASN:HD21	13	0.12
(1,3098)	1:B:15:LYS:HD3	1:B:16:ASN:HD21	13	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	3	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	3	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	5	0.12
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	5	0.12
(1,2790)	1:B:50:MET:HG3	1:B:51:ILE:H	17	0.12
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	4	0.12
(1,278)	1:B:20:ASN:H	1:B:20:ASN:HD22	18	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG21	12	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG22	12	0.12
(1,2629)	1:A:9:ARG:HE	1:A:46:THR:HG23	12	0.12
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	4	0.12
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	4	0.12
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	4	0.12
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	19	0.12
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	19	0.12
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	19	0.12
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	15	0.12
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	19	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD11	4	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD12	4	0.12
(1,2311)	1:A:35:THR:HB	1:A:36:ILE:HD13	4	0.12
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	18	0.12
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	18	0.12
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	18	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	10	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	10	0.12
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	10	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	5	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	7	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	7	0.12
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	7	0.12
(1,2164)	1:B:27:SER:HG	1:B:28:LYS:HG2	5	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	1	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	5	0.12
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	15	0.12
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	9	0.12
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	13	0.12
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG21	1:B:65:LYS:HE3	15	0.12
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG22	1:B:65:LYS:HE3	15	0.12
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE2	15	0.12
(1,1813)	1:B:25:VAL:HG23	1:B:65:LYS:HE3	15	0.12
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG21	1:A:41:LYS:HE3	11	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG22	1:A:41:LYS:HE3	11	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE2	11	0.12
(1,1808)	1:A:11:VAL:HG23	1:A:41:LYS:HE3	11	0.12
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	2	0.12
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	2	0.12
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	2	0.12
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	3	0.12
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	3	0.12
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	3	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD21	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD11	1:B:62:LEU:HD23	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD21	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD12	1:B:62:LEU:HD23	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD21	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD22	18	0.12
(1,1538)	1:B:8:ILE:HD13	1:B:62:LEU:HD23	18	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	10	0.12
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	10	0.12
(1,718)	1:A:41:LYS:H	1:A:46:THR:H	11	0.11
(1,545)	1:A:29:PHE:HD1	1:A:31:THR:H	3	0.11
(1,545)	1:A:29:PHE:HD2	1:A:31:THR:H	3	0.11
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB2	10	0.11
(1,4940)	1:B:55:ASN:HD21	1:B:57:ASP:HB3	10	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB2	10	0.11
(1,4940)	1:B:55:ASN:HD22	1:B:57:ASP:HB3	10	0.11
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB2	20	0.11
(1,4896)	1:B:39:ASN:HD21	1:B:41:LYS:HB3	20	0.11
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB2	20	0.11
(1,4896)	1:B:39:ASN:HD22	1:B:41:LYS:HB3	20	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	5	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	5	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD21	17	0.11
(1,4885)	1:B:37:VAL:HG11	1:B:39:ASN:HD22	17	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD21	17	0.11
(1,4885)	1:B:37:VAL:HG12	1:B:39:ASN:HD22	17	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD21	17	0.11
(1,4885)	1:B:37:VAL:HG13	1:B:39:ASN:HD22	17	0.11
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG21	1:B:28:LYS:HG3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG22	1:B:28:LYS:HG3	19	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG2	19	0.11
(1,4815)	1:B:25:VAL:HG23	1:B:28:LYS:HG3	19	0.11
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB2	9	0.11
(1,4770)	1:B:15:LYS:HD2	1:B:16:ASN:HB3	9	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB2	9	0.11
(1,4770)	1:B:15:LYS:HD3	1:B:16:ASN:HB3	9	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE1	14	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE2	14	0.11
(1,4623)	1:A:48:ASN:HD21	1:A:50:MET:HE3	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE1	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE2	14	0.11
(1,4623)	1:A:48:ASN:HD22	1:A:50:MET:HE3	14	0.11
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB2	20	0.11
(1,4602)	1:A:39:ASN:HD21	1:A:41:LYS:HB3	20	0.11
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB2	20	0.11
(1,4602)	1:A:39:ASN:HD22	1:A:41:LYS:HB3	20	0.11
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG11	1:A:39:ASN:HD22	13	0.11
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG12	1:A:39:ASN:HD22	13	0.11
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD21	13	0.11
(1,4591)	1:A:37:VAL:HG13	1:A:39:ASN:HD22	13	0.11
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB2	8	0.11
(1,4459)	1:A:15:LYS:HG2	1:A:16:ASN:HB3	8	0.11
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB2	8	0.11
(1,4459)	1:A:15:LYS:HG3	1:A:16:ASN:HB3	8	0.11
(1,4400)	1:A:81:LEU:HD11	1:A:83:HIS:HE1	20	0.11
(1,4400)	1:A:81:LEU:HD12	1:A:83:HIS:HE1	20	0.11
(1,4400)	1:A:81:LEU:HD13	1:A:83:HIS:HE1	20	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG11	4	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG12	4	0.11
(1,4374)	1:A:4:PHE:HE1	1:A:53:VAL:HG13	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG11	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG12	4	0.11
(1,4374)	1:A:4:PHE:HE2	1:A:53:VAL:HG13	4	0.11
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE1	12	0.11
(1,4333)	1:B:4:PHE:HB2	1:B:52:PHE:HE2	12	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE1	12	0.11
(1,4333)	1:B:4:PHE:HB3	1:B:52:PHE:HE2	12	0.11
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4209)	1:B:29:PHE:HA	1:B:29:PHE:HD2	4	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	10	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	11	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	12	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	15	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG11	19	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG12	19	0.11
(1,4177)	1:B:4:PHE:HZ	1:B:53:VAL:HG13	19	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	15	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG11	17	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG12	17	0.11
(1,4176)	1:A:4:PHE:HZ	1:A:53:VAL:HG13	17	0.11
(1,4072)	1:A:60:THR:HB	1:A:61:THR:H	2	0.11
(1,4053)	1:B:41:LYS:HG2	1:B:42:ASP:HA	1	0.11
(1,4053)	1:B:41:LYS:HG3	1:B:42:ASP:HA	1	0.11
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	4	0.11
(1,4037)	1:B:15:LYS:HA	1:B:17:GLY:H	10	0.11
(1,4036)	1:A:15:LYS:HA	1:A:17:GLY:H	12	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG21	20	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG22	20	0.11
(1,3702)	1:B:11:VAL:H	1:B:74:THR:HG23	20	0.11
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	2	0.11
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	15	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	15	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	15	0.11
(1,3680)	1:B:72:VAL:HG11	1:B:74:THR:HB	19	0.11
(1,3680)	1:B:72:VAL:HG12	1:B:74:THR:HB	19	0.11
(1,3680)	1:B:72:VAL:HG13	1:B:74:THR:HB	19	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	1	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	1	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	2	0.11
(1,3679)	1:A:72:VAL:HG11	1:A:74:THR:HB	3	0.11
(1,3679)	1:A:72:VAL:HG12	1:A:74:THR:HB	3	0.11
(1,3679)	1:A:72:VAL:HG13	1:A:74:THR:HB	3	0.11
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE2	15	0.11
(1,3558)	1:B:15:LYS:H	1:B:15:LYS:HE3	15	0.11
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE2	7	0.11
(1,3557)	1:A:15:LYS:H	1:A:15:LYS:HE3	7	0.11
(1,3483)	1:A:41:LYS:HE2	1:A:44:ILE:H	1	0.11
(1,3483)	1:A:41:LYS:HE3	1:A:44:ILE:H	1	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE1	19	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE2	19	0.11
(1,3407)	1:B:61:THR:HA	1:B:63:MET:HE3	19	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE1	16	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE2	16	0.11
(1,3406)	1:A:61:THR:HA	1:A:63:MET:HE3	16	0.11
(1,3149)	1:A:55:ASN:H	1:A:58:LYS:HB2	6	0.11
(1,3103)	1:A:54:LYS:HE2	1:A:55:ASN:HD21	1	0.11
(1,3103)	1:A:54:LYS:HE3	1:A:55:ASN:HD21	1	0.11
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE2	17	0.11
(1,3101)	1:A:54:LYS:HA	1:A:54:LYS:HE3	17	0.11
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD2	18	0.11
(1,3099)	1:A:54:LYS:H	1:A:54:LYS:HD3	18	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG11	15	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG12	15	0.11
(1,2989)	1:A:4:PHE:HB2	1:A:53:VAL:HG13	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG11	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG12	15	0.11
(1,2989)	1:A:4:PHE:HB3	1:A:53:VAL:HG13	15	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	2	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	2	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	2	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	7	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	7	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD11	1:B:58:LYS:HZ3	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD12	1:B:58:LYS:HZ3	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ1	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ2	8	0.11
(1,2948)	1:B:51:ILE:HD13	1:B:58:LYS:HZ3	8	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD11	1:A:58:LYS:HZ3	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD12	1:A:58:LYS:HZ3	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ1	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ2	19	0.11
(1,2947)	1:A:51:ILE:HD13	1:A:58:LYS:HZ3	19	0.11
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	1	0.11
(1,2598)	1:B:44:ILE:HD11	1:B:45:PHE:H	15	0.11
(1,2598)	1:B:44:ILE:HD12	1:B:45:PHE:H	15	0.11
(1,2598)	1:B:44:ILE:HD13	1:B:45:PHE:H	15	0.11
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	8	0.11
(1,2597)	1:A:44:ILE:HD11	1:A:45:PHE:H	12	0.11
(1,2597)	1:A:44:ILE:HD12	1:A:45:PHE:H	12	0.11
(1,2597)	1:A:44:ILE:HD13	1:A:45:PHE:H	12	0.11
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	4	0.11
(1,2548)	1:B:40:ALA:HA	1:B:44:ILE:HG13	18	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	3	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	16	0.11
(1,2547)	1:A:40:ALA:HA	1:A:44:ILE:HG13	18	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	4	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	5	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	9	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	15	0.11
(1,2304)	1:B:36:ILE:HG21	1:B:48:ASN:H	16	0.11
(1,2304)	1:B:36:ILE:HG22	1:B:48:ASN:H	16	0.11
(1,2304)	1:B:36:ILE:HG23	1:B:48:ASN:H	16	0.11
(1,2303)	1:A:36:ILE:HG21	1:A:48:ASN:H	8	0.11
(1,2303)	1:A:36:ILE:HG22	1:A:48:ASN:H	8	0.11
(1,2303)	1:A:36:ILE:HG23	1:A:48:ASN:H	8	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD11	7	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD12	7	0.11
(1,230)	1:A:19:THR:H	1:A:38:LEU:HD13	7	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG21	12	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG22	12	0.11
(1,2286)	1:B:23:THR:HB	1:B:36:ILE:HG23	12	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG21	18	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG22	18	0.11
(1,2285)	1:A:23:THR:HB	1:A:36:ILE:HG23	18	0.11
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG21	1:B:39:ASN:HB3	10	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG22	1:B:39:ASN:HB3	10	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB2	10	0.11
(1,2284)	1:A:36:ILE:HG23	1:B:39:ASN:HB3	10	0.11
(1,2173)	1:A:68:LYS:HA	1:A:68:LYS:HD2	6	0.11
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	8	0.11
(1,1840)	1:B:18:MET:HA	1:B:21:GLN:HA	12	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	1	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	5	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	7	0.11
(1,1839)	1:A:18:MET:HA	1:A:21:GLN:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG21	20	0.11
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG22	20	0.11
(1,1815)	1:B:68:LYS:HE2	1:B:69:VAL:HG23	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG21	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG22	20	0.11
(1,1815)	1:B:68:LYS:HE3	1:B:69:VAL:HG23	20	0.11
(1,1795)	1:B:14:ASP:HA	1:B:15:LYS:HB3	8	0.11
(1,175)	1:A:15:LYS:H	1:A:18:MET:HG2	15	0.11
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	7	0.11
(1,1695)	1:B:11:VAL:HG21	1:B:40:ALA:HA	10	0.11
(1,1695)	1:B:11:VAL:HG22	1:B:40:ALA:HA	10	0.11
(1,1695)	1:B:11:VAL:HG23	1:B:40:ALA:HA	10	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	1	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	8	0.11
(1,1694)	1:A:11:VAL:HG21	1:A:40:ALA:HA	18	0.11
(1,1694)	1:A:11:VAL:HG22	1:A:40:ALA:HA	18	0.11
(1,1694)	1:A:11:VAL:HG23	1:A:40:ALA:HA	18	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD11	1:A:62:LEU:HD23	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD12	1:A:62:LEU:HD23	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD21	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD22	15	0.11
(1,1537)	1:A:8:ILE:HD13	1:A:62:LEU:HD23	15	0.11
(1,1413)	1:A:3:ASP:HB2	1:A:53:VAL:H	1	0.11
(1,1318)	1:B:77:ARG:HG2	1:B:78:LEU:H	8	0.11
(1,1020)	1:A:58:LYS:HZ1	1:A:61:THR:H	20	0.11
(1,1020)	1:A:58:LYS:HZ2	1:A:61:THR:H	20	0.11
(1,1020)	1:A:58:LYS:HZ3	1:A:61:THR:H	20	0.11

10 Dihedral-anlge violation analysis

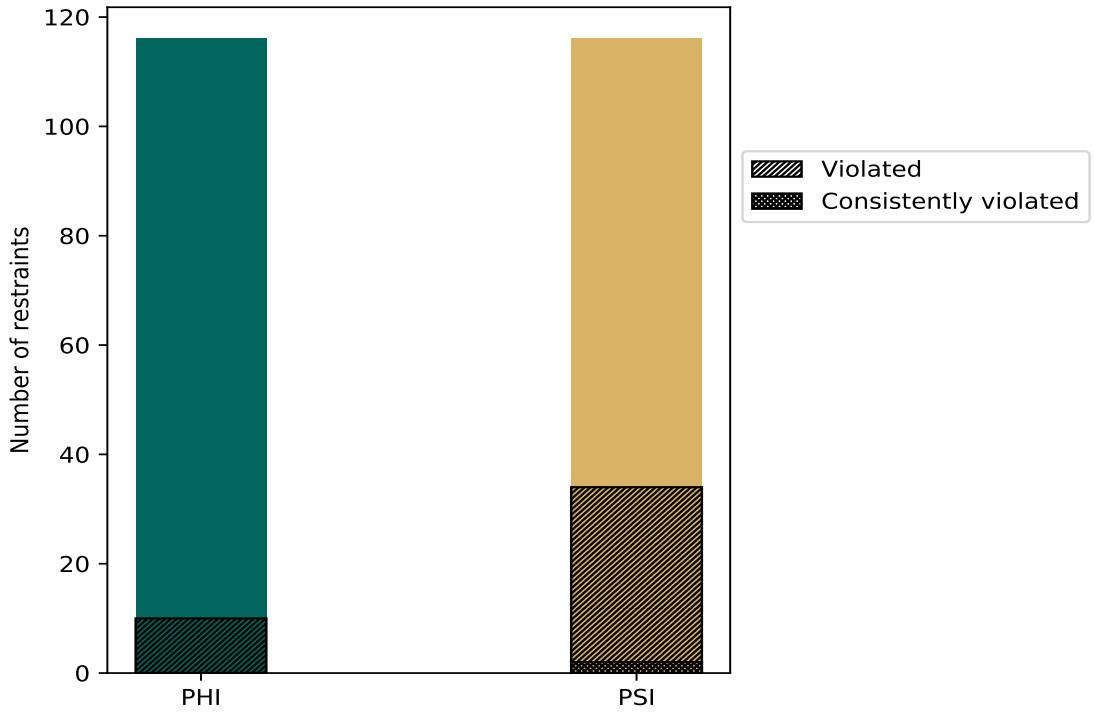
10.1 Summary of dihedral-anlge violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	116	50.0	10	8.6	4.3	0	0.0	0.0
PSI	116	50.0	34	29.3	14.7	2	1.7	0.9
Total	232	100.0	44	19.0	19.0	2	0.9	0.9

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

10.1.1 Bar chart : Distribution of dihedral-anlges and violations



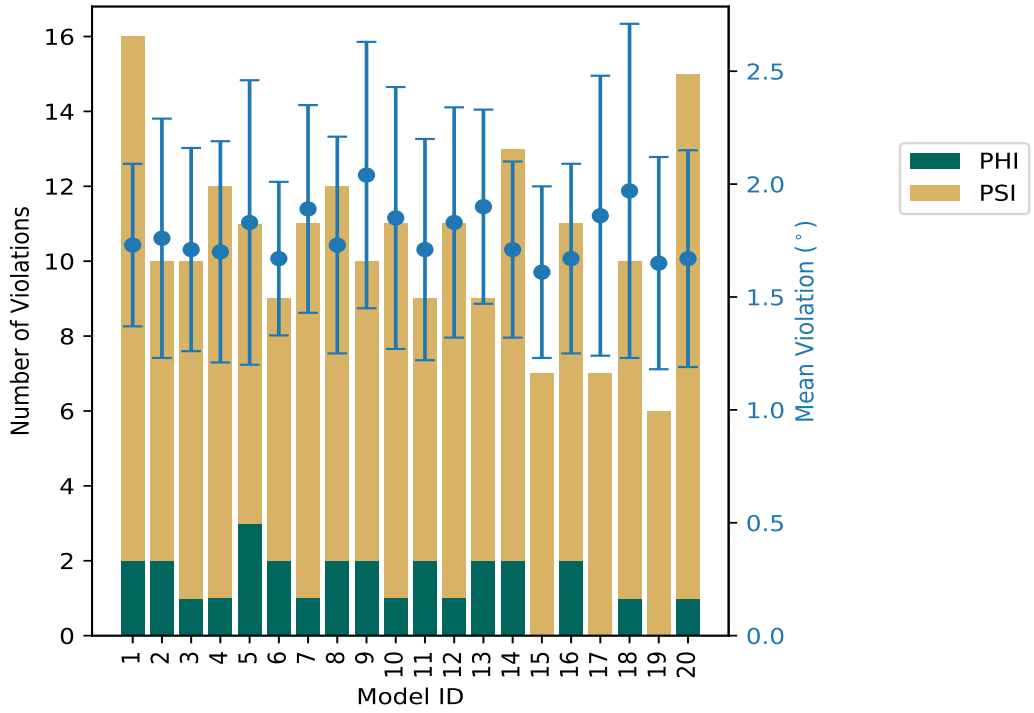
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-anlge violation statistics in each model

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

Model ID	Number of violations			Mean (°)	Max (°)	Std. deviation (°)
	PHI	PSI	Total			
1	2	14	16	1.73	2.3	0.36
2	2	8	10	1.76	2.7	0.53
3	1	9	10	1.71	2.4	0.45
4	1	11	12	1.7	2.7	0.49
5	3	8	11	1.83	3.0	0.63
6	2	7	9	1.67	2.3	0.34
7	1	10	11	1.89	2.4	0.46
8	2	10	12	1.73	2.7	0.48
9	2	8	10	2.04	2.7	0.59
10	1	10	11	1.85	3.0	0.58
11	2	7	9	1.71	2.8	0.49
12	1	10	11	1.83	2.6	0.51
13	2	7	9	1.9	2.4	0.43
14	2	11	13	1.71	2.4	0.39
15	0	7	7	1.61	2.2	0.38
16	2	9	11	1.67	2.6	0.42
17	0	7	7	1.86	3.0	0.62
18	1	9	10	1.97	3.6	0.74
19	0	6	6	1.65	2.4	0.47
20	1	14	15	1.67	2.5	0.48

10.2.1 Bar graph : Dihedral violation statistics for each model



The mean and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Violation statistics in the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
4	15	19	1	5.0
2	0	2	2	10.0
1	5	6	3	15.0
1	1	2	4	20.0
1	0	1	5	25.0
0	3	3	6	30.0
0	1	1	7	35.0
1	0	1	8	40.0
0	0	0	9	45.0
0	2	2	10	50.0
0	2	2	11	55.0
0	1	1	12	60.0

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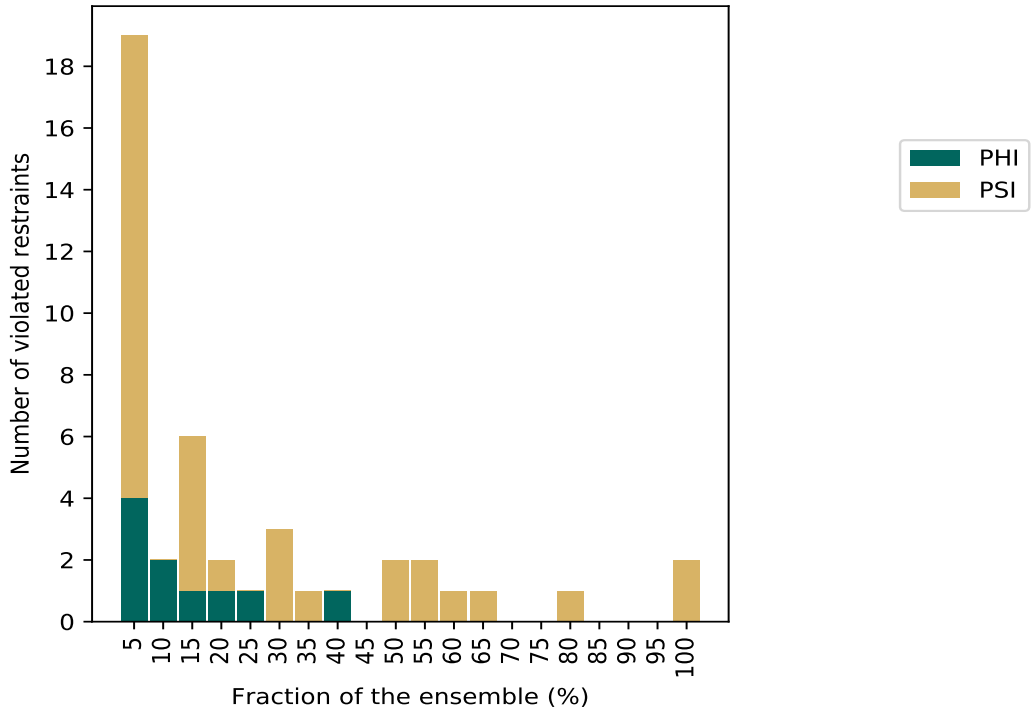
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	2	2	20	100.0

[1] Number of models with violations

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

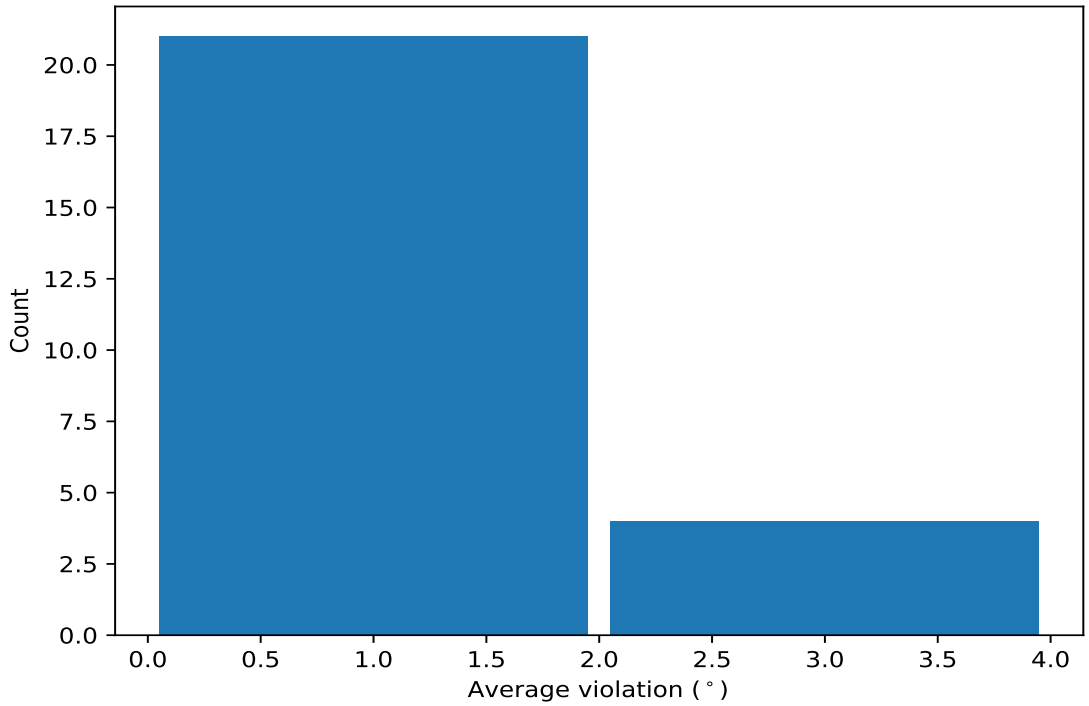


10.4 Most violated dihedral-anlge restraints

10.4.1 Histogram : Distribution of mean dihedral-anlge violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-anlge restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean (°)	SD[2] (°)
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	11	2.29	0.68
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	16	1.96	0.43
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	20	2.06	0.52
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	20	2.17	0.41
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	10	1.74	0.58
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	10	1.89	0.39
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	13	1.71	0.44
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	12	1.7	0.46
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	11	1.71	0.38
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	3	1.6	0.45
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	3	1.67	0.39
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	6	1.77	0.36
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	4	1.68	0.43
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	6	1.68	0.36
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	6	1.32	0.28
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	7	1.5	0.3
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	3	1.4	0.24
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	3	1.23	0.19
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	3	1.4	0.08
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	4	2.13	0.29

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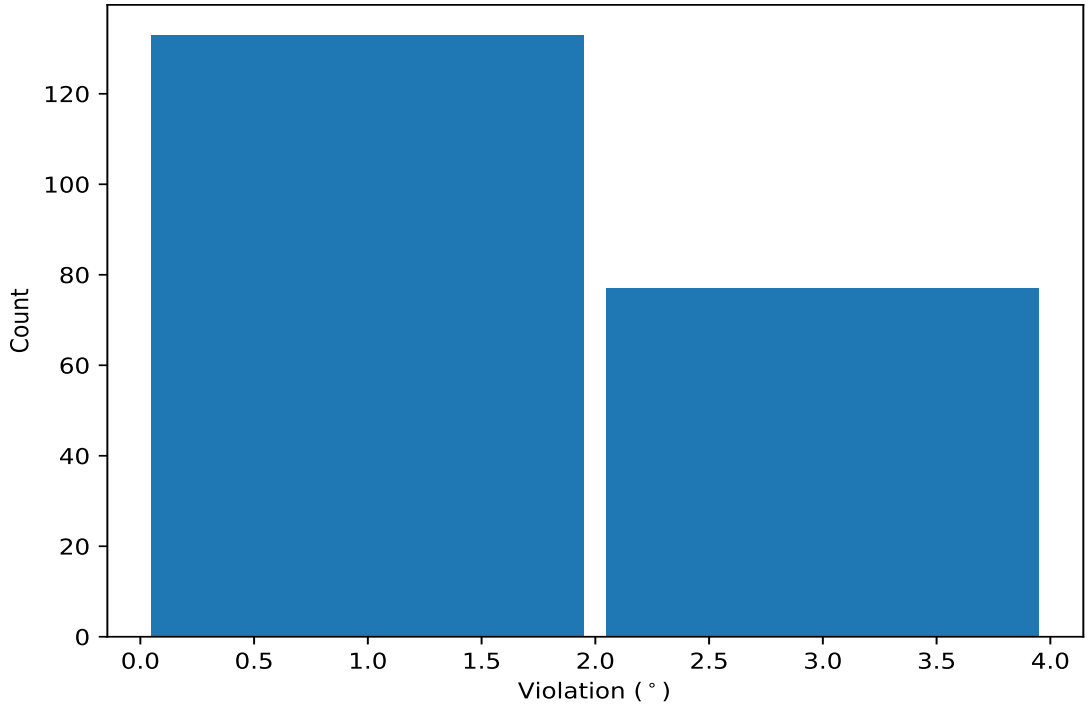
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean (°)	SD[2] (°)
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	8	1.55	0.34
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	3	1.6	0.41
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	2	1.85	0.15
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	5	1.44	0.27
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	2	1.1	0.0

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

10.5 All violated dihedral-anlge restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-anlge restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	18	3.6
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	10	3.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	5	3.0
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	17	3.0
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	18	2.9
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	11	2.8
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	9	2.7
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	2	2.7
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	8	2.7
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	2	2.7
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	4	2.7
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	9	2.6
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	9	2.6
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	10	2.6
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	12	2.6
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	16	2.6
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	20	2.5
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	9	2.5
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	4	2.5
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	3	2.4
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	5	2.4
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	12	2.4
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	19	2.4
(1,20)	1:A:14:ASP:N	1:A:14:ASP:CA	1:A:14:ASP:C	1:A:15:LYS:N	7	2.4
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	8	2.4
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	13	2.4
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	17	2.4
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	12	2.4
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	14	2.4
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	7	2.4
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	20	2.4
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	13	2.4
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	1	2.3
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	7	2.3
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	6	2.3
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	14	2.3
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	5	2.3
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	5	2.3
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	7	2.3
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	3	2.3
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	12	2.3
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	7	2.2
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	9	2.2
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	18	2.2
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	14	2.2
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	20	2.2
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	10	2.2
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	15	2.2
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	16	2.2
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	20	2.2
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	1	2.2
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	8	2.1
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	1	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	10	2.1
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	13	2.1
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	15	2.1
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	8	2.1
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	3	2.1
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	10	2.1
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	18	2.1
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	7	2.1
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	1	2.1
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	3	2.1
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	11	2.1
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	19	2.1
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	9	2.1
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	9	2.1
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	5	2.1
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	5	2.1
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	4	2.0
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	20	2.0
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	1	2.0
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	14	2.0
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	13	2.0
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	13	2.0
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	13	2.0
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	20	2.0
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	4	1.9
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	16	1.9
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	17	1.9
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	12	1.9
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	1	1.9
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	13	1.9
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	6	1.9
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	2	1.9
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	4	1.9
(1,136)	1:B:14:ASP:N	1:B:14:ASP:CA	1:B:14:ASP:C	1:B:15:LYS:N	6	1.9
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	1	1.9
(1,71)	1:A:48:ASN:C	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	6	1.8
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	1	1.8
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	2	1.8
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	8	1.8
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	11	1.8
(1,221)	1:B:67:ARG:C	1:B:68:LYS:N	1:B:68:LYS:CA	1:B:68:LYS:C	7	1.8
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	11	1.8
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	16	1.8
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	18	1.8
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	17	1.8
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	2	1.7
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	6	1.7
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	14	1.7
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	18	1.7
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	1	1.7
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	11	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	8	1.7
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	14	1.7
(1,201)	1:B:57:ASP:C	1:B:58:LYS:N	1:B:58:LYS:CA	1:B:58:LYS:C	2	1.7
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	12	1.7
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	15	1.7
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	16	1.7
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	19	1.7
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	10	1.7
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	12	1.7
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	3	1.7
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	11	1.6
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	18	1.6
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	14	1.6
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	1	1.6
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	16	1.6
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	14	1.6
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	14	1.6
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	17	1.6
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	18	1.6
(1,139)	1:B:17:GLY:C	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	6	1.6
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	4	1.6
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	10	1.6
(1,96)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:ASP:N	1	1.5
(1,60)	1:A:40:ALA:N	1:A:40:ALA:CA	1:A:40:ALA:C	1:A:41:LYS:N	7	1.5
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	20	1.5
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	20	1.5
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	1	1.5
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	4	1.5
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	3	1.5
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	12	1.5
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	16	1.5
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	15	1.5
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	14	1.4
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	8	1.4
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	10	1.4
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	7	1.4
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	4	1.4
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	9	1.4
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	1	1.4
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	8	1.4
(1,138)	1:B:15:LYS:N	1:B:15:LYS:CA	1:B:15:LYS:C	1:B:16:ASN:N	3	1.4
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	2	1.4
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	15	1.4
(1,128)	1:B:9:ARG:N	1:B:9:ARG:CA	1:B:9:ARG:C	1:B:10:ILE:N	20	1.4
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	2	1.4
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	4	1.4
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	8	1.4
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	16	1.4
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	5	1.3
(1,28)	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	1:A:21:GLN:N	6	1.3
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	16	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	8	1.3
(1,220)	1:B:67:ARG:N	1:B:67:ARG:CA	1:B:67:ARG:C	1:B:68:LYS:N	11	1.3
(1,22)	1:A:15:LYS:N	1:A:15:LYS:CA	1:A:15:LYS:C	1:A:16:ASN:N	15	1.3
(1,212)	1:B:63:MET:N	1:B:63:MET:CA	1:B:63:MET:C	1:B:64:ASP:N	19	1.3
(1,204)	1:B:59:LEU:N	1:B:59:LEU:CA	1:B:59:LEU:C	1:B:60:THR:N	20	1.3
(1,182)	1:B:46:THR:N	1:B:46:THR:CA	1:B:46:THR:C	1:B:47:CYS:N	8	1.3
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	12	1.3
(1,148)	1:B:22:ILE:N	1:B:22:ILE:CA	1:B:22:ILE:C	1:B:23:THR:N	7	1.3
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	10	1.3
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	19	1.3
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	20	1.3
(1,14)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1:A:11:VAL:N	6	1.3
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	20	1.3
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	1	1.3
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	14	1.3
(1,90)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:THR:N	3	1.2
(1,54)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:LEU:N	6	1.2
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	11	1.2
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	17	1.2
(1,23)	1:A:17:GLY:C	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	5	1.2
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	4	1.2
(1,228)	1:B:75:VAL:N	1:B:75:VAL:CA	1:B:75:VAL:C	1:B:76:GLU:N	14	1.2
(1,196)	1:B:53:VAL:N	1:B:53:VAL:CA	1:B:53:VAL:C	1:B:54:LYS:N	12	1.2
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	4	1.2
(1,171)	1:B:37:VAL:C	1:B:38:LEU:N	1:B:38:LEU:CA	1:B:38:LEU:C	5	1.2
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	3	1.2
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	20	1.2
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	2	1.2
(1,140)	1:B:18:MET:N	1:B:18:MET:CA	1:B:18:MET:C	1:B:19:THR:N	16	1.2
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	3	1.2
(1,12)	1:A:9:ARG:N	1:A:9:ARG:CA	1:A:9:ARG:C	1:A:10:ILE:N	13	1.2
(1,112)	1:A:75:VAL:N	1:A:75:VAL:CA	1:A:75:VAL:C	1:A:76:GLU:N	10	1.2
(1,110)	1:A:74:THR:N	1:A:74:THR:CA	1:A:74:THR:C	1:A:75:VAL:N	14	1.2
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	16	1.2
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	1	1.2
(1,88)	1:A:59:LEU:N	1:A:59:LEU:CA	1:A:59:LEU:C	1:A:60:THR:N	1	1.1
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	8	1.1
(1,85)	1:A:57:ASP:C	1:A:58:LYS:N	1:A:58:LYS:CA	1:A:58:LYS:C	11	1.1
(1,55)	1:A:37:VAL:C	1:A:38:LEU:N	1:A:38:LEU:CA	1:A:38:LEU:C	9	1.1
(1,42)	1:A:27:SER:N	1:A:27:SER:CA	1:A:27:SER:C	1:A:28:LYS:N	12	1.1
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	5	1.1
(1,34)	1:A:23:THR:N	1:A:23:THR:CA	1:A:23:THR:C	1:A:24:GLY:N	18	1.1
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	13	1.1
(1,32)	1:A:22:ILE:N	1:A:22:ILE:CA	1:A:22:ILE:C	1:A:23:THR:N	15	1.1
(1,27)	1:A:19:THR:C	1:A:20:ASN:N	1:A:20:ASN:CA	1:A:20:ASN:C	20	1.1
(1,24)	1:A:18:MET:N	1:A:18:MET:CA	1:A:18:MET:C	1:A:19:THR:N	19	1.1
(1,170)	1:B:37:VAL:N	1:B:37:VAL:CA	1:B:37:VAL:C	1:B:38:LEU:N	20	1.1
(1,166)	1:B:35:THR:N	1:B:35:THR:CA	1:B:35:THR:C	1:B:36:ILE:N	4	1.1
(1,158)	1:B:27:SER:N	1:B:27:SER:CA	1:B:27:SER:C	1:B:28:LYS:N	10	1.1
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	5	1.1
(1,150)	1:B:23:THR:N	1:B:23:THR:CA	1:B:23:THR:C	1:B:24:GLY:N	9	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:B:10:ILE:N	1:B:10:ILE:CA	1:B:10:ILE:C	1:B:11:VAL:N	7	1.1
(1,120)	1:B:5:LEU:N	1:B:5:LEU:CA	1:B:5:LEU:C	1:B:6:ALA:N	17	1.1
(1,105)	1:A:67:ARG:C	1:A:68:LYS:N	1:A:68:LYS:CA	1:A:68:LYS:C	18	1.1
(1,104)	1:A:67:ARG:N	1:A:67:ARG:CA	1:A:67:ARG:C	1:A:68:LYS:N	2	1.1