wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2JUW
Title	:	NMR solution structure of homodimer protein SO_2176 from Shewanella oneidensis. Northeast Structural Genomics Consortium target SoR77
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Deposited on	:	2007-09-03

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

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

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

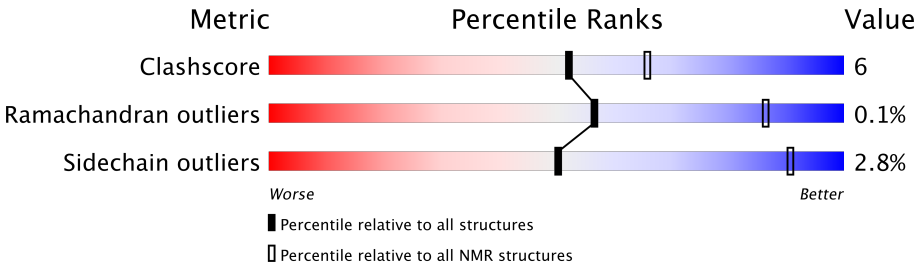
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analalysis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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 66%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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

Mol	Chain	Length	Quality of chain
1	A	80	69% 10% 21%
1	B	80	73% 8% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:70, B:8-B:71 (127)	0.48	8

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2542 atoms, of which 1288 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UPF0352 protein SO_2176.

Mol	Chain	Residues	Atoms						Trace
1	A	80	Total	C	H	N	O	S	0
			1271	391	644	116	117	3	
1	B	80	Total	C	H	N	O	S	0
			1271	391	644	116	117	3	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	LEU	-	EXPRESSION TAG	UNP Q8EF26
A	74	GLU	-	EXPRESSION TAG	UNP Q8EF26
A	75	HIS	-	EXPRESSION TAG	UNP Q8EF26
A	76	HIS	-	EXPRESSION TAG	UNP Q8EF26
A	77	HIS	-	EXPRESSION TAG	UNP Q8EF26
A	78	HIS	-	EXPRESSION TAG	UNP Q8EF26
A	79	HIS	-	EXPRESSION TAG	UNP Q8EF26
A	80	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	73	LEU	-	EXPRESSION TAG	UNP Q8EF26
B	74	GLU	-	EXPRESSION TAG	UNP Q8EF26
B	75	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	76	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	77	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	78	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	79	HIS	-	EXPRESSION TAG	UNP Q8EF26
B	80	HIS	-	EXPRESSION TAG	UNP Q8EF26

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

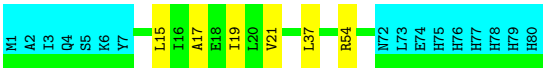
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain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

• Molecule 1: UPF0352 protein SO_2176

Chain A:

• Molecule 1: UPF0352 protein SO_2176

Chain B:



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

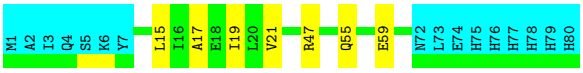
The representative model is number 8. Colouring as in section 4.1 above.

• Molecule 1: UPF0352 protein SO_2176

Chain A:

• Molecule 1: UPF0352 protein SO_2176

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: *structures with the lowest energy.*

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

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

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

Chemical shift file(s)	2juw_nmr.cif
Number of chemical shift lists	1
Total number of shifts	1959
Number of shifts mapped to atoms	1217
Number of unparsed shifts	278
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	464
Assignment completeness (well-defined parts)	66%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	478	506	504	8±2
1	B	484	511	509	7±2
All	All	19240	20340	20260	245

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ALA:HB1	1:B:62:ALA:HB1	0.73	1.60	7	3
1:B:48:LYS:HE2	1:B:48:LYS:HA	0.70	1.63	16	1
1:B:45:LEU:HB3	1:B:54:ARG:HG3	0.69	1.63	4	6
1:B:15:LEU:O	1:B:19:ILE:HG12	0.64	1.93	4	2
1:A:15:LEU:O	1:A:19:ILE:HG12	0.63	1.93	2	5

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	63/80 (79%)	62±1 (98±2%)	1±1 (1±2%)	0±0 (0±0%)	56 86
1	B	64/80 (80%)	63±1 (99±2%)	1±1 (1±2%)	0±0 (0±0%)	56 86
All	All	2540/3200 (79%)	2506 (99%)	32 (1%)	2 (0%)	56 86

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	8	SER	1
1	B	8	SER	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	54/70 (77%)	53±1 (98±2%)	1±1 (2±2%)	54 92
1	B	55/70 (79%)	53±1 (97±2%)	2±1 (3±2%)	48 89
All	All	2180/2800 (78%)	2120 (97%)	60 (3%)	50 91

5 of 35 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	43	HIS	5
1	B	47	ARG	4
1	A	24	GLU	3
1	B	63	LYS	3
1	B	52	GLU	3

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: 2juw_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_2juw_rt.mr*

7.1.1 Bookkeeping

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

Total number of shifts	1959
Number of shifts mapped to atoms	1217
Number of unparsed shifts	278
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	464
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 278) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	A	2	ALA	HB%	1.510	0.020	1
4	A	2	ALA	HB%	1.510	0.020	1
12	A	3	ILE	HD1%	0.870	0.020	1
13	A	3	ILE	HD1%	0.870	0.020	1
17	A	3	ILE	HG2%	0.920	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 464) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	ILE	HG1y	1.78	0.02	2
B	31	ASP	HBy	2.88	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	59	GLU	HGx	2.32	0.02	2
B	39	ASN	HBy	2.85	0.02	2
B	55	GLN	HG%	2.32	0.02	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	154	-0.56 ± 0.08	Should be applied
$^{13}C_{\beta}$	152	0.24 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	148	-0.39 ± 0.10	None needed (< 0.5 ppm)
^{15}N	148	0.31 ± 0.22	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 1012 atoms were assigned a chemical shift out of a possible 1532. 32 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	621/627 (99%)	248/250 (99%)	250/254 (98%)	123/123 (100%)
Sidechain	363/855 (42%)	46/496 (9%)	301/325 (93%)	16/34 (47%)
Aromatic	28/50 (56%)	12/26 (46%)	12/16 (75%)	4/8 (50%)
Overall	1012/1532 (66%)	306/772 (40%)	563/595 (95%)	143/165 (87%)

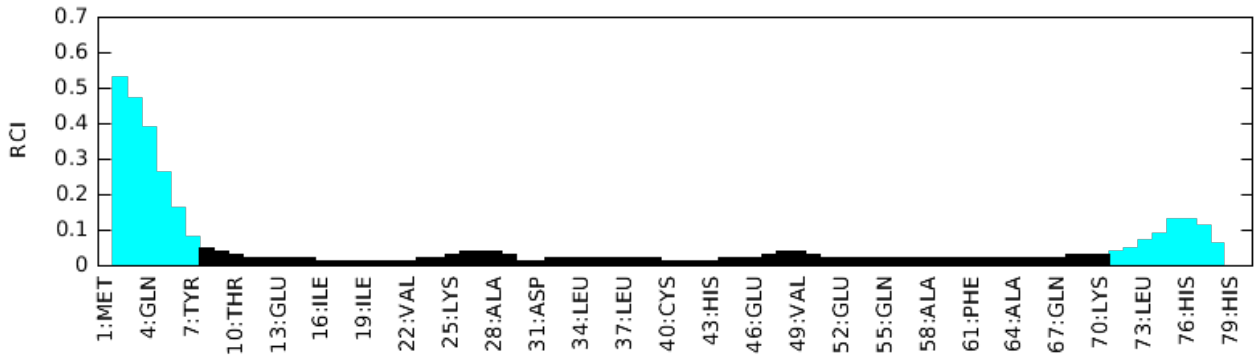
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

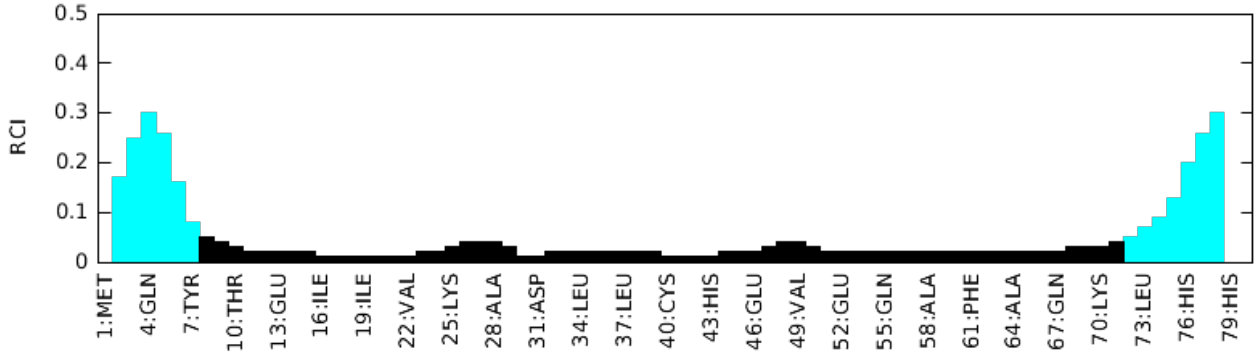
7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 Distance restraints analysis

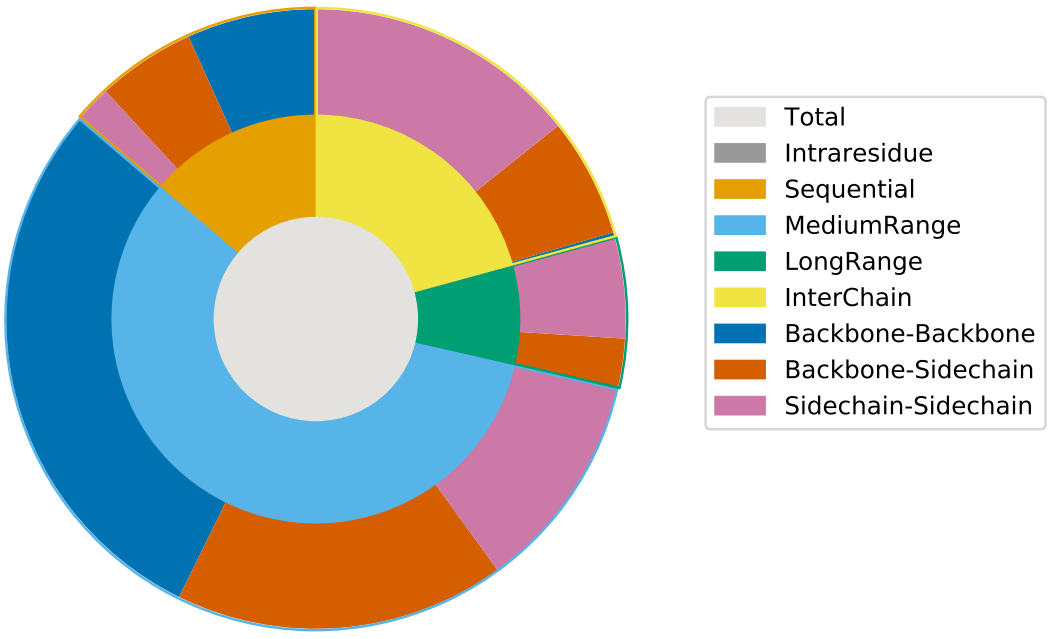
8.1 Distance restraints summary

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

Restraints type	B-B[1](H[4])	B-S[2](H[4])	S-S[3](H[4])	Total		
				Total(H[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0)	0(0)	0(0)	0(0)	0.0	0.0
Sequential (|i-j|=1)	100(0)	76(0)	28(0)	204(0)	1.4	13.7
Medium range (|i-j|>1 and |i-j|<5)	430(122)	256(0)	170(0)	856(122)	5.9	57.7
Long range (|i-j|≥5)	0(0)	38(0)	78(0)	116(0)	0.8	7.8
Inter chain	4(0)	92(0)	212(0)	308(0)	2.1	20.8
Total	534(122)	462(0)	488(0)	1484(122)	10.3	100.0

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

8.1.1 Pie chart : Distance restraints summary



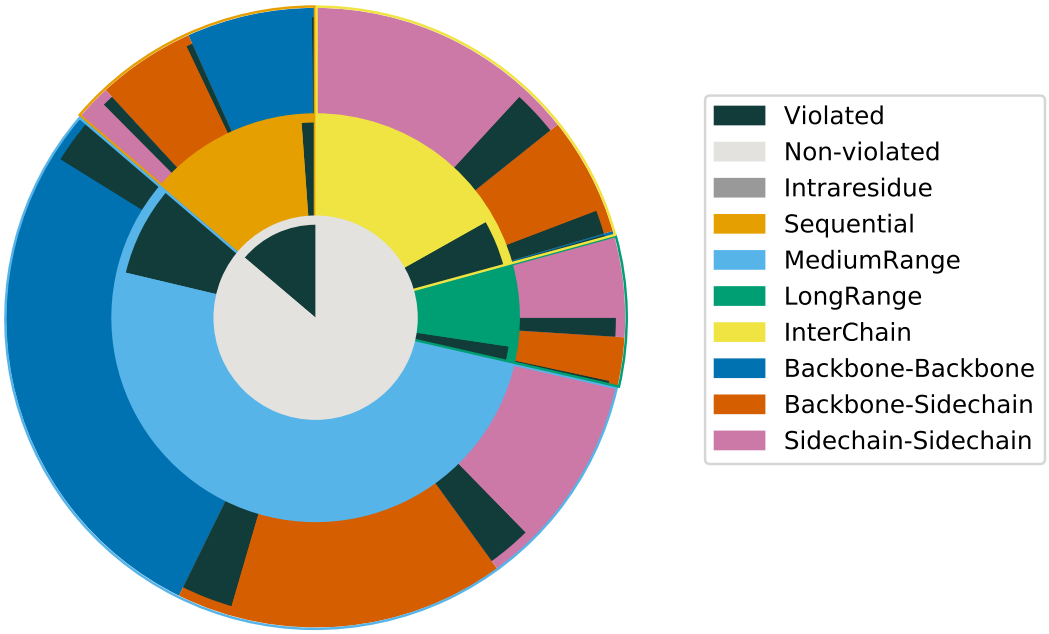
8.2 Distance violations summary

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

Restraints type	B-B[1](%[4])	B-S[2](%[4])	S-S[3](%[4])	Total		
				Total(%[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Sequential (|i-j|=1)	3(3.0)	5(6.6)	9(32.1)	17(8.3)	0.1	8.3
Medium range (|i-j|>1 and |i-j|<5)	36(8.4)	41(16.0)	35(20.6)	112(13.1)	0.8	54.6
Long range (|i-j|≥5)	0(0.0)	3(7.9)	15(19.2)	18(15.5)	0.1	8.8
Inter chain	3(75.0)	19(20.7)	36(17.0)	58(18.8)	0.4	28.3
Total	42(7.9)	68(14.7)	95(19.5)	205(13.8)	1.4	100.0

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

8.2.1 Pie-chart : Distance violations summary



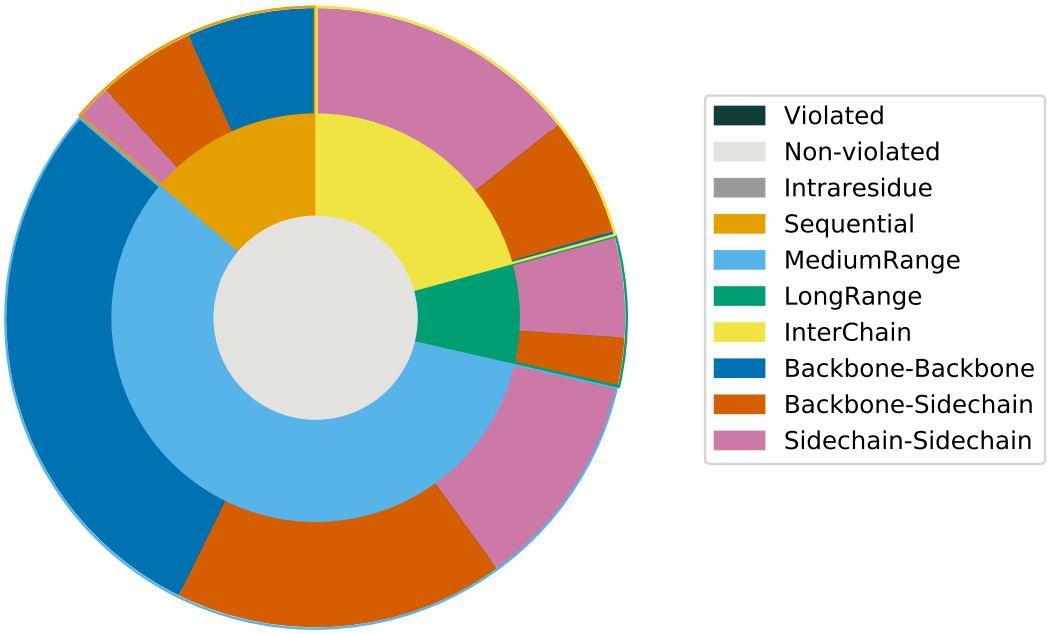
8.3 Consistent distance violations summary

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

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

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

8.3.1 Pie-chart : Consistent distance violations



8.4 Residual distance violations

Violation are counted in different bin sizes and listed below

Range (Å)	Avg. No. of violated restraints per model	Max violation (Å)
0-0.2	25.6	0.03
0.2-0.5	None	None
0.5-1.0	None	None
1.0-2.0	None	None
2.0-5.0	None	None
5.0<	None	None

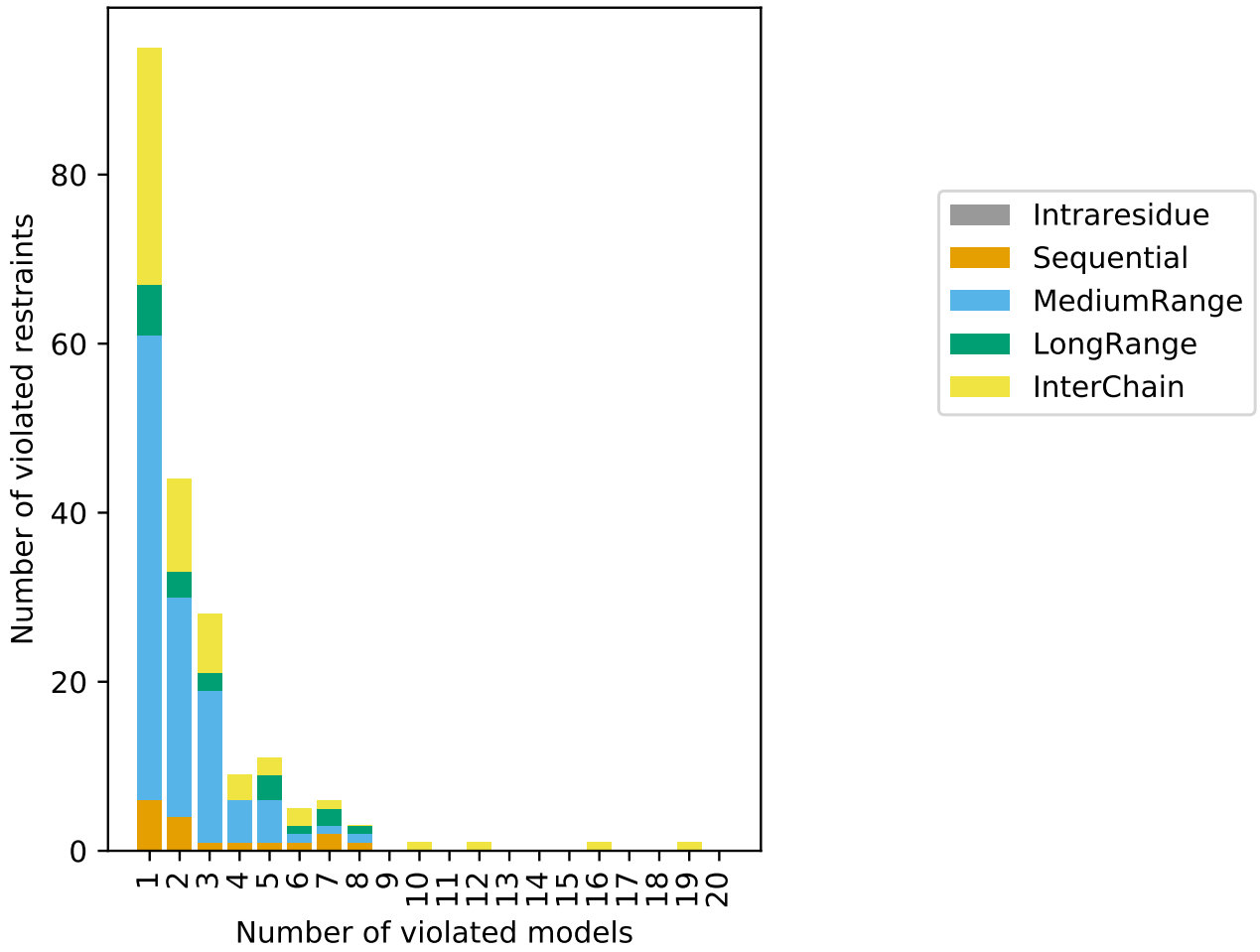
8.5 Distance violations in ensemble

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

No. of violated restraints						No. of violated models
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	
0	6	55	6	28	95	1
0	4	26	3	11	44	2
0	1	18	2	7	28	3
0	1	5	0	3	9	4
0	1	5	3	2	11	5
0	1	1	1	2	5	6
0	2	1	2	1	6	7
0	1	1	1	0	3	8
0	0	0	0	0	0	9
0	0	0	0	1	1	10
0	0	0	0	0	0	11
0	0	0	0	1	1	12
0	0	0	0	0	0	13
0	0	0	0	0	0	14
0	0	0	0	0	0	15
0	0	0	0	1	1	16
0	0	0	0	0	0	17
0	0	0	0	0	0	18
0	0	0	0	1	1	19
0	0	0	0	0	0	20

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

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



0 intraresidue restraints, 187 sequential restraints, 744 medium range restraints,98 long range restraints and 250 inter chain restraints are not violated. In total, 1279 restraints are not violated in any of the models

8.6 Violations in each model

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

Model ID	No. of violations						Mean (Å)	Max (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total		
1	0	5	12	2	5	24	0.01	0.02
2	0	2	9	3	9	23	0.01	0.02
3	0	5	9	4	7	25	0.01	0.03
4	0	0	11	2	11	24	0.01	0.03
5	0	2	11	2	8	23	0.01	0.02

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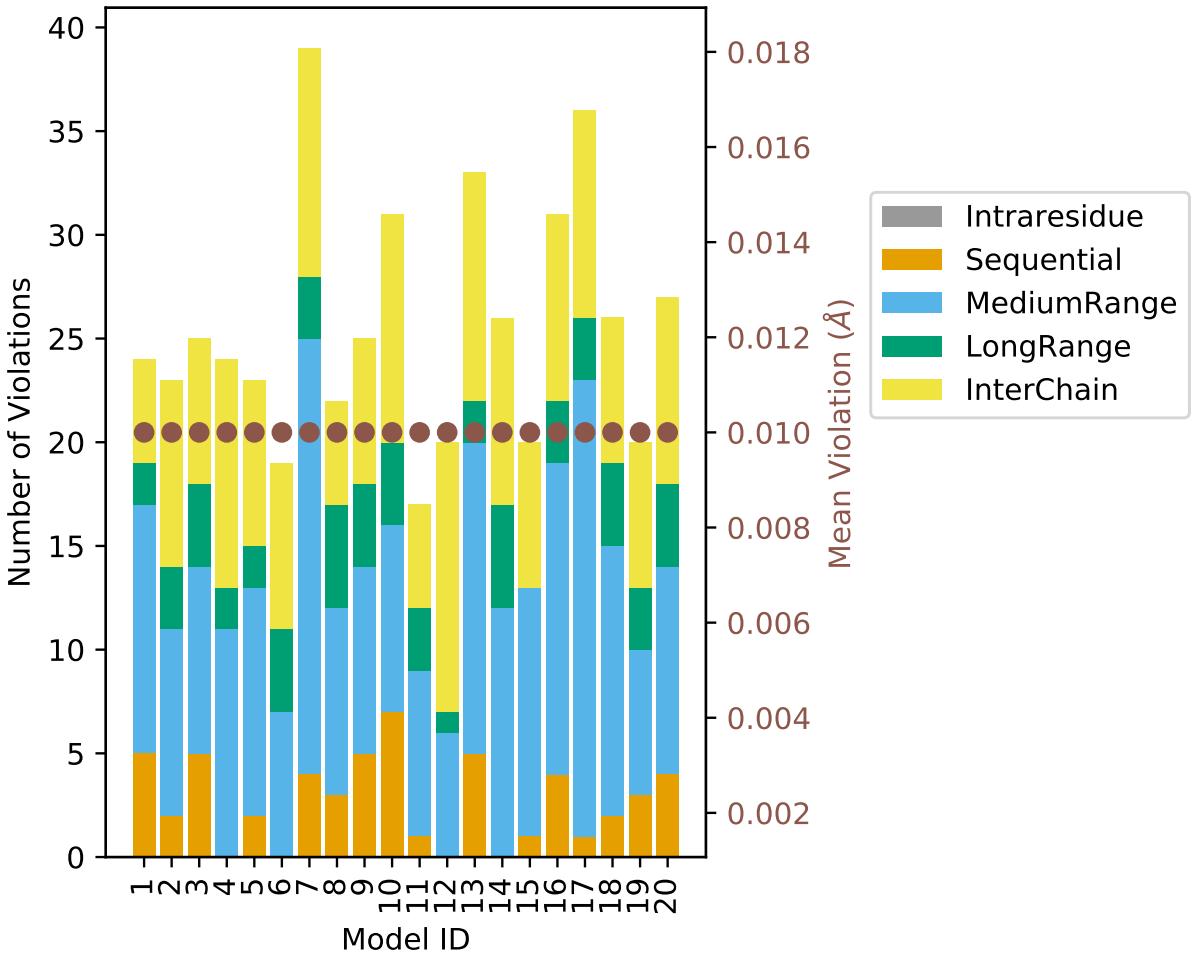
Model ID	No. of violations						Mean (Å)	Max (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total		
6	0	0	7	4	8	19	0.01	0.03
7	0	4	21	3	11	39	0.01	0.02
8	0	3	9	5	5	22	0.01	0.03
9	0	5	9	4	7	25	0.01	0.03
10	0	7	9	4	11	31	0.01	0.03
11	0	1	8	3	5	17	0.01	0.02
12	0	0	6	1	13	20	0.01	0.02
13	0	5	15	2	11	33	0.01	0.03
14	0	0	12	5	9	26	0.01	0.02
15	0	1	12	0	7	20	0.01	0.03
16	0	4	15	3	9	31	0.01	0.02
17	0	1	22	3	10	36	0.01	0.03
18	0	2	13	4	7	26	0.01	0.02
19	0	3	7	3	7	20	0.01	0.02
20	0	4	10	4	9	27	0.01	0.02

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

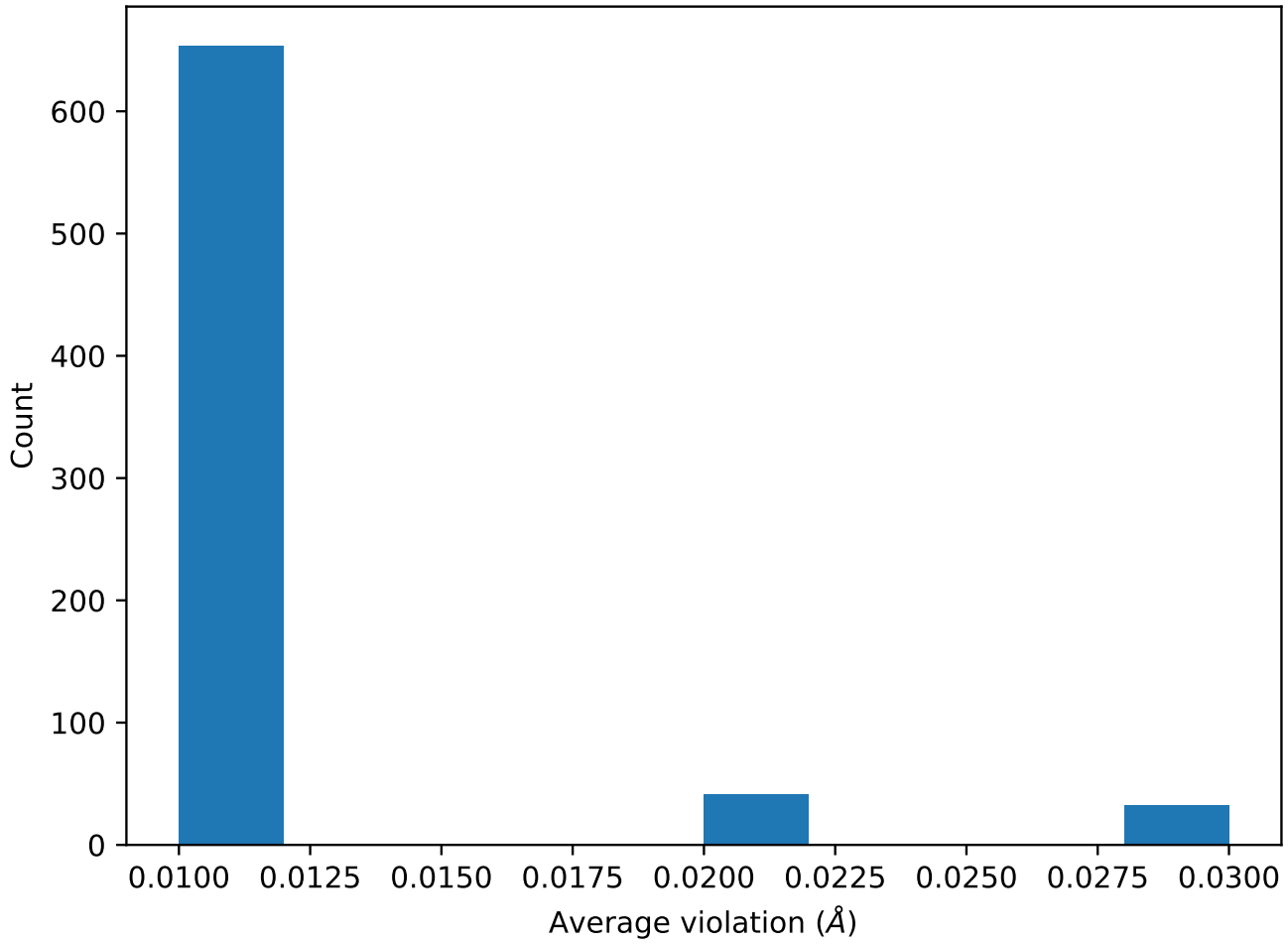
8.6.1 Bar graph : Violations in each model



8.7 Most violated distance restraints

8.7.1 Histogram : Distribution of mean distance violations

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



8.7.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	19	0.02	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	19	0.02	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	19	0.02	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	16	0.01	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	16	0.01	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	16	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	12	0.01	0.02
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	12	0.01	0.02
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	12	0.01	0.02
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	12	0.01	0.02
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	12	0.01	0.02
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	12	0.01	0.02
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	10	0.01	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	10	0.01	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	10	0.01	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	10	0.01	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	10	0.01	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	10	0.01	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	8	0.01	0.02
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	8	0.01	0.02
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	8	0.01	0.02
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	8	0.01	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	8	0.01	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	8	0.01	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	7	0.01	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	7	0.01	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	7	0.01	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	7	0.01	0.02
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	7	0.01	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	7	0.01	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	7	0.01	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	7	0.01	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	7	0.01	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	7	0.01	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	7	0.01	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	7	0.01	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	7	0.01	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	7	0.01	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	7	0.01	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	7	0.01	0.03
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	7	0.01	0.03
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	7	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	7	0.01	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	7	0.01	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	6	0.01	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	6	0.01	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	6	0.01	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	6	0.01	0.02
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	6	0.01	0.02
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	6	0.01	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	6	0.01	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	6	0.01	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	6	0.01	0.02
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	6	0.01	0.02
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	6	0.01	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	6	0.01	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	6	0.01	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	6	0.01	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	6	0.01	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	6	0.01	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	6	0.01	0.02
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	5	0.01	0.02
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	5	0.01	0.02
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	5	0.01	0.02
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	5	0.01	0.02
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	5	0.01	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	5	0.01	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	5	0.01	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	5	0.01	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	5	0.01	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	5	0.01	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	5	0.01	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	5	0.01	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	5	0.01	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	5	0.01	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	5	0.01	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	5	0.01	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	5	0.01	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	5	0.01	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	5	0.01	0.01
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	5	0.01	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	5	0.01	0.02
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	5	0.01	0.02
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	5	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	5	0.01	0.02
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	5	0.01	0.02
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	5	0.01	0.02
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	5	0.01	0.01
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	5	0.01	0.02
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	5	0.01	0.02
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	5	0.01	0.02
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	5	0.01	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	5	0.01	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	5	0.01	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	5	0.01	0.01
(1,971)	1:B:23:LEU:HA	1:B:26:HIS:HD2	4	0.01	0.02
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE2	4	0.01	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE3	4	0.01	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE2	4	0.01	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE3	4	0.01	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE2	4	0.01	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE3	4	0.01	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG21	4	0.01	0.02
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG22	4	0.01	0.02
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG23	4	0.01	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG21	4	0.01	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG22	4	0.01	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG23	4	0.01	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG21	4	0.01	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG22	4	0.01	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG23	4	0.01	0.02
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG2	4	0.01	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG3	4	0.01	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG2	4	0.01	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG3	4	0.01	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG2	4	0.01	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG3	4	0.01	0.01
(1,698)	1:A:51:SER:HB2	1:A:54:ARG:HE	4	0.01	0.01
(1,698)	1:A:51:SER:HB3	1:A:54:ARG:HE	4	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD11	4	0.01	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD12	4	0.01	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD13	4	0.01	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD1	4	0.01	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD2	4	0.01	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD1	4	0.01	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD2	4	0.01	0.01
(1,243)	1:B:34:LEU:HA	1:A:41:VAL:HA	4	0.01	0.01
(1,237)	1:B:30:THR:HG21	1:A:48:LYS:HA	4	0.01	0.01
(1,237)	1:B:30:THR:HG22	1:A:48:LYS:HA	4	0.01	0.01
(1,237)	1:B:30:THR:HG23	1:A:48:LYS:HA	4	0.01	0.01
(1,973)	1:B:23:LEU:HA	1:B:27:LYS:H	3	0.01	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG21	3	0.01	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG22	3	0.01	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG23	3	0.01	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG21	3	0.01	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG22	3	0.01	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG23	3	0.01	0.01
(1,89)	1:A:34:LEU:HA	1:B:41:VAL:HA	3	0.01	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD11	3	0.01	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD12	3	0.01	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD13	3	0.01	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	3	0.01	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	3	0.01	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	3	0.01	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	3	0.01	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	3	0.01	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	3	0.01	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB2	3	0.01	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB3	3	0.01	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB2	3	0.01	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB3	3	0.01	0.01
(1,808)	1:A:65:LEU:HB2	1:A:68:SER:H	3	0.01	0.01
(1,808)	1:A:65:LEU:HB3	1:A:68:SER:H	3	0.01	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB1	3	0.01	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB2	3	0.01	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB3	3	0.01	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB1	3	0.01	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB2	3	0.01	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB3	3	0.01	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD2	3	0.01	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD3	3	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,446)	1:A:23:LEU:HA	1:A:27:LYS:H	3	0.01	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	3	0.01	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	3	0.01	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	3	0.01	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	3	0.01	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	3	0.01	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	3	0.01	0.01
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD1	3	0.02	0.03
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD2	3	0.02	0.03
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD1	3	0.02	0.03
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD2	3	0.02	0.03
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG21	3	0.01	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG22	3	0.01	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG23	3	0.01	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG21	3	0.01	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG22	3	0.01	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG23	3	0.01	0.01
(1,207)	1:B:16:ILE:HG21	1:A:43:HIS:HD2	3	0.01	0.01
(1,207)	1:B:16:ILE:HG22	1:A:43:HIS:HD2	3	0.01	0.01
(1,207)	1:B:16:ILE:HG23	1:A:43:HIS:HD2	3	0.01	0.01
(1,173)	1:B:11:GLN:HG2	1:A:32:LEU:HG	3	0.01	0.01
(1,173)	1:B:11:GLN:HG3	1:A:32:LEU:HG	3	0.01	0.01
(1,1483)	1:B:69:VAL:H	1:B:65:LEU:O	3	0.01	0.01
(1,1443)	1:B:23:LEU:H	1:B:19:ILE:O	3	0.01	0.02
(1,1421)	1:A:69:VAL:H	1:A:65:LEU:O	3	0.01	0.01
(1,1389)	1:A:35:MET:H	1:A:31:ASP:O	3	0.01	0.01
(1,1388)	1:A:25:LYS:N	1:A:21:VAL:O	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD21	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD22	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD23	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD21	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD22	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD23	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD21	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD22	3	0.01	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD23	3	0.01	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB2	3	0.01	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB3	3	0.01	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB2	3	0.01	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB3	3	0.01	0.01
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG2	3	0.01	0.02
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG3	3	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG2	3	0.01	0.02
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG3	3	0.01	0.02
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG2	3	0.01	0.02
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG3	3	0.01	0.02
(1,126)	1:A:42:THR:HG21	1:B:65:LEU:HG	3	0.01	0.02
(1,126)	1:A:42:THR:HG22	1:B:65:LEU:HG	3	0.01	0.02
(1,126)	1:A:42:THR:HG23	1:B:65:LEU:HG	3	0.01	0.02
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD11	3	0.01	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD12	3	0.01	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD13	3	0.01	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB2	3	0.01	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB3	3	0.01	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB2	3	0.01	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB3	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE1	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE2	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE3	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE1	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE2	3	0.01	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE3	3	0.01	0.01
(1,1003)	1:B:26:HIS:HB3	1:B:28:ALA:H	3	0.02	0.03
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB1	2	0.01	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB2	2	0.01	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB3	2	0.01	0.01
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE1	2	0.02	0.03
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE2	2	0.02	0.03
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE1	2	0.02	0.03
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE2	2	0.02	0.03
(1,836)	1:B:5:SER:HA	1:B:7:TYR:H	2	0.01	0.02
(1,83)	1:A:30:THR:HG21	1:B:48:LYS:HA	2	0.01	0.01
(1,83)	1:A:30:THR:HG22	1:B:48:LYS:HA	2	0.01	0.01
(1,83)	1:A:30:THR:HG23	1:B:48:LYS:HA	2	0.01	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD21	2	0.01	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD22	2	0.01	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB2	2	0.01	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB3	2	0.01	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB2	2	0.01	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB3	2	0.01	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB2	2	0.01	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB3	2	0.01	0.01
(1,773)	1:A:60:GLN:HB2	1:A:62:ALA:H	2	0.01	0.01
(1,773)	1:A:60:GLN:HB3	1:A:62:ALA:H	2	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD2	2	0.01	0.02
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD3	2	0.01	0.02
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB1	2	0.01	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB2	2	0.01	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB3	2	0.01	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB1	2	0.01	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB2	2	0.01	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB3	2	0.01	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE2	2	0.01	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE3	2	0.01	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE2	2	0.01	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE3	2	0.01	0.01
(1,73)	1:A:20:LEU:HD11	1:B:43:HIS:HE1	2	0.01	0.01
(1,73)	1:A:20:LEU:HD12	1:B:43:HIS:HE1	2	0.01	0.01
(1,73)	1:A:20:LEU:HD13	1:B:43:HIS:HE1	2	0.01	0.01
(1,696)	1:A:51:SER:HB2	1:A:53:SER:H	2	0.01	0.02
(1,696)	1:A:51:SER:HB3	1:A:53:SER:H	2	0.01	0.02
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD2	2	0.01	0.01
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD3	2	0.01	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD2	2	0.01	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD3	2	0.01	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD2	2	0.01	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD3	2	0.01	0.01
(1,599)	1:A:41:VAL:HA	1:A:45:LEU:H	2	0.01	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG21	2	0.01	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG22	2	0.01	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG23	2	0.01	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG21	2	0.01	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG22	2	0.01	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG23	2	0.01	0.01
(1,561)	1:A:37:LEU:HB2	1:A:41:VAL:H	2	0.03	0.03
(1,561)	1:A:37:LEU:HB3	1:A:41:VAL:H	2	0.03	0.03
(1,53)	1:A:16:ILE:HG21	1:B:43:HIS:HD2	2	0.01	0.01
(1,53)	1:A:16:ILE:HG22	1:B:43:HIS:HD2	2	0.01	0.01
(1,53)	1:A:16:ILE:HG23	1:B:43:HIS:HD2	2	0.01	0.01
(1,444)	1:A:23:LEU:HA	1:A:26:HIS:HD2	2	0.01	0.01
(1,340)	1:A:10:THR:HG21	1:A:14:SER:H	2	0.01	0.01
(1,340)	1:A:10:THR:HG22	1:A:14:SER:H	2	0.01	0.01
(1,340)	1:A:10:THR:HG23	1:A:14:SER:H	2	0.01	0.01
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE1	2	0.01	0.02
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE2	2	0.01	0.02
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE1	2	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE2	2	0.01	0.02
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG2	2	0.01	0.01
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG3	2	0.01	0.01
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG2	2	0.01	0.01
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG3	2	0.01	0.01
(1,280)	1:B:42:THR:HG21	1:A:65:LEU:HG	2	0.01	0.02
(1,280)	1:B:42:THR:HG22	1:A:65:LEU:HG	2	0.01	0.02
(1,280)	1:B:42:THR:HG23	1:A:65:LEU:HG	2	0.01	0.02
(1,254)	1:B:37:LEU:HD11	1:A:41:VAL:HB	2	0.01	0.01
(1,254)	1:B:37:LEU:HD12	1:A:41:VAL:HB	2	0.01	0.01
(1,254)	1:B:37:LEU:HD13	1:A:41:VAL:HB	2	0.01	0.01
(1,219)	1:B:19:ILE:HD11	1:A:37:LEU:H	2	0.01	0.01
(1,219)	1:B:19:ILE:HD12	1:A:37:LEU:H	2	0.01	0.01
(1,219)	1:B:19:ILE:HD13	1:A:37:LEU:H	2	0.01	0.01
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG11	2	0.01	0.02
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG12	2	0.01	0.02
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG13	2	0.01	0.02
(1,202)	1:B:16:ILE:HG12	1:A:39:ASN:H	2	0.01	0.01
(1,202)	1:B:16:ILE:HG13	1:A:39:ASN:H	2	0.01	0.01
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE1	2	0.01	0.02
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE2	2	0.01	0.02
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE3	2	0.01	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE1	2	0.01	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE2	2	0.01	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE3	2	0.01	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE1	2	0.01	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE2	2	0.01	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE3	2	0.01	0.02
(1,1448)	1:B:25:LYS:N	1:B:21:VAL:O	2	0.01	0.01
(1,1435)	1:B:19:ILE:H	1:B:15:LEU:O	2	0.01	0.01
(1,1406)	1:A:61:PHE:N	1:A:57:VAL:O	2	0.01	0.01
(1,1375)	1:A:19:ILE:H	1:A:15:LEU:O	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB1	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB2	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB3	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB1	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB2	2	0.01	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB3	2	0.01	0.01
(1,1301)	1:B:60:GLN:HB2	1:B:63:LYS:H	2	0.01	0.01
(1,1301)	1:B:60:GLN:HB3	1:B:63:LYS:H	2	0.01	0.01
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD2	2	0.01	0.02
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD3	2	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1276)	1:B:57:VAL:HG11	1:B:61:PHE:H	2	0.01	0.01
(1,1276)	1:B:57:VAL:HG12	1:B:61:PHE:H	2	0.01	0.01
(1,1276)	1:B:57:VAL:HG13	1:B:61:PHE:H	2	0.01	0.01
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB1	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB2	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB3	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB1	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB2	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB3	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB1	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB2	2	0.03	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB3	2	0.03	0.03
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB2	2	0.01	0.01
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB3	2	0.01	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB2	2	0.01	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB3	2	0.01	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB2	2	0.01	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB3	2	0.01	0.01
(1,1225)	1:B:51:SER:HB2	1:B:54:ARG:HE	2	0.01	0.01
(1,1225)	1:B:51:SER:HB3	1:B:54:ARG:HE	2	0.01	0.01
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG2	2	0.01	0.02
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG3	2	0.01	0.02
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG2	2	0.01	0.02
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG3	2	0.01	0.02
(1,1153)	1:B:43:HIS:HD2	1:B:44:LEU:HG	2	0.01	0.01
(1,1150)	1:B:43:HIS:HA	1:B:47:ARG:H	2	0.01	0.01
(1,1114)	1:B:40:CYS:HA	1:B:43:HIS:HD2	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB2	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB3	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB2	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB3	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB2	2	0.01	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB3	2	0.01	0.01
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD21	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD22	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD23	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD21	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD22	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD23	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD21	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD22	2	0.01	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD23	2	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,995)	1:B:24:GLU:HB2	1:B:26:HIS:H	1	0.01	0.01
(1,995)	1:B:24:GLU:HB3	1:B:26:HIS:H	1	0.01	0.01
(1,966)	1:B:22:VAL:HG21	1:B:25:LYS:HE2	1	0.01	0.01
(1,966)	1:B:22:VAL:HG21	1:B:25:LYS:HE3	1	0.01	0.01
(1,966)	1:B:22:VAL:HG22	1:B:25:LYS:HE2	1	0.01	0.01
(1,966)	1:B:22:VAL:HG22	1:B:25:LYS:HE3	1	0.01	0.01
(1,966)	1:B:22:VAL:HG23	1:B:25:LYS:HE2	1	0.01	0.01
(1,966)	1:B:22:VAL:HG23	1:B:25:LYS:HE3	1	0.01	0.01
(1,963)	1:B:22:VAL:HG11	1:B:25:LYS:HB2	1	0.01	0.01
(1,963)	1:B:22:VAL:HG11	1:B:25:LYS:HB3	1	0.01	0.01
(1,963)	1:B:22:VAL:HG12	1:B:25:LYS:HB2	1	0.01	0.01
(1,963)	1:B:22:VAL:HG12	1:B:25:LYS:HB3	1	0.01	0.01
(1,963)	1:B:22:VAL:HG13	1:B:25:LYS:HB2	1	0.01	0.01
(1,963)	1:B:22:VAL:HG13	1:B:25:LYS:HB3	1	0.01	0.01
(1,840)	1:B:6:LYS:HD2	1:B:7:TYR:HD1	1	0.01	0.01
(1,840)	1:B:6:LYS:HD2	1:B:7:TYR:HD2	1	0.01	0.01
(1,840)	1:B:6:LYS:HD3	1:B:7:TYR:HD1	1	0.01	0.01
(1,840)	1:B:6:LYS:HD3	1:B:7:TYR:HD2	1	0.01	0.01
(1,835)	1:A:72:ASN:H	1:A:73:LEU:HB2	1	0.01	0.01
(1,835)	1:A:72:ASN:H	1:A:73:LEU:HB3	1	0.01	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD11	1	0.01	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD12	1	0.01	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD13	1	0.01	0.01
(1,829)	1:A:69:VAL:H	1:A:70:LYS:HB2	1	0.01	0.01
(1,829)	1:A:69:VAL:H	1:A:70:LYS:HB3	1	0.01	0.01
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD21	1	0.01	0.01
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD22	1	0.01	0.01
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD23	1	0.01	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD21	1	0.01	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD22	1	0.01	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD23	1	0.01	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD21	1	0.01	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD22	1	0.01	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD23	1	0.01	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG21	1	0.01	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG22	1	0.01	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG23	1	0.01	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG21	1	0.01	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG22	1	0.01	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG23	1	0.01	0.01
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG21	1	0.01	0.01
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG22	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG23	1	0.01	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD21	1	0.01	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD22	1	0.01	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD23	1	0.01	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD21	1	0.01	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD22	1	0.01	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD23	1	0.01	0.01
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD21	1	0.01	0.01
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD22	1	0.01	0.01
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD23	1	0.01	0.01
(1,780)	1:A:61:PHE:HD1	1:A:65:LEU:HB2	1	0.01	0.01
(1,780)	1:A:61:PHE:HD1	1:A:65:LEU:HB3	1	0.01	0.01
(1,780)	1:A:61:PHE:HD2	1:A:65:LEU:HB2	1	0.01	0.01
(1,780)	1:A:61:PHE:HD2	1:A:65:LEU:HB3	1	0.01	0.01
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD11	1	0.02	0.02
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD12	1	0.02	0.02
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD13	1	0.02	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD11	1	0.02	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD12	1	0.02	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD13	1	0.02	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD11	1	0.02	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD12	1	0.02	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD13	1	0.02	0.02
(1,774)	1:A:60:GLN:HB2	1:A:63:LYS:H	1	0.01	0.01
(1,774)	1:A:60:GLN:HB3	1:A:63:LYS:H	1	0.01	0.01
(1,749)	1:A:57:VAL:HG11	1:A:61:PHE:H	1	0.01	0.01
(1,749)	1:A:57:VAL:HG12	1:A:61:PHE:H	1	0.01	0.01
(1,749)	1:A:57:VAL:HG13	1:A:61:PHE:H	1	0.01	0.01
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB1	1	0.03	0.03
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB2	1	0.03	0.03
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB3	1	0.03	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB1	1	0.03	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB2	1	0.03	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB3	1	0.03	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB1	1	0.03	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB2	1	0.03	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB3	1	0.03	0.03
(1,658)	1:A:46:GLU:HG2	1:A:54:ARG:HE	1	0.01	0.01
(1,658)	1:A:46:GLU:HG3	1:A:54:ARG:HE	1	0.01	0.01
(1,623)	1:A:43:HIS:HA	1:A:47:ARG:H	1	0.01	0.01
(1,621)	1:A:42:THR:HG21	1:A:46:GLU:H	1	0.01	0.01
(1,621)	1:A:42:THR:HG22	1:A:46:GLU:H	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,621)	1:A:42:THR:HG23	1:A:46:GLU:H	1	0.01	0.01
(1,619)	1:A:42:THR:HA	1:A:46:GLU:H	1	0.01	0.01
(1,616)	1:A:42:THR:HA	1:A:45:LEU:HB2	1	0.01	0.01
(1,616)	1:A:42:THR:HA	1:A:45:LEU:HB3	1	0.01	0.01
(1,60)	1:A:19:ILE:HD11	1:B:22:VAL:HB	1	0.01	0.01
(1,60)	1:A:19:ILE:HD12	1:B:22:VAL:HB	1	0.01	0.01
(1,60)	1:A:19:ILE:HD13	1:B:22:VAL:HB	1	0.01	0.01
(1,595)	1:A:41:VAL:HA	1:A:44:LEU:HB2	1	0.01	0.01
(1,589)	1:A:40:CYS:HB2	1:A:43:HIS:HB2	1	0.02	0.02
(1,589)	1:A:40:CYS:HB2	1:A:43:HIS:HB3	1	0.02	0.02
(1,589)	1:A:40:CYS:HB3	1:A:43:HIS:HB2	1	0.02	0.02
(1,589)	1:A:40:CYS:HB3	1:A:43:HIS:HB3	1	0.02	0.02
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG11	1	0.01	0.01
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG12	1	0.01	0.01
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG13	1	0.01	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG21	1	0.01	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG22	1	0.01	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG23	1	0.01	0.01
(1,562)	1:A:37:LEU:HD11	1:A:40:CYS:HB2	1	0.01	0.01
(1,562)	1:A:37:LEU:HD11	1:A:40:CYS:HB3	1	0.01	0.01
(1,562)	1:A:37:LEU:HD12	1:A:40:CYS:HB2	1	0.01	0.01
(1,562)	1:A:37:LEU:HD12	1:A:40:CYS:HB3	1	0.01	0.01
(1,562)	1:A:37:LEU:HD13	1:A:40:CYS:HB2	1	0.01	0.01
(1,562)	1:A:37:LEU:HD13	1:A:40:CYS:HB3	1	0.01	0.01
(1,550)	1:A:35:MET:HB2	1:A:39:ASN:HD21	1	0.01	0.01
(1,550)	1:A:35:MET:HB2	1:A:39:ASN:HD22	1	0.01	0.01
(1,550)	1:A:35:MET:HB3	1:A:39:ASN:HD21	1	0.01	0.01
(1,550)	1:A:35:MET:HB3	1:A:39:ASN:HD22	1	0.01	0.01
(1,547)	1:A:34:LEU:H	1:A:37:LEU:H	1	0.01	0.01
(1,546)	1:A:34:LEU:H	1:A:37:LEU:HB2	1	0.01	0.01
(1,546)	1:A:34:LEU:H	1:A:37:LEU:HB3	1	0.01	0.01
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE1	1	0.01	0.01
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE2	1	0.01	0.01
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE3	1	0.01	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE1	1	0.01	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE2	1	0.01	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE3	1	0.01	0.01
(1,482)	1:A:27:LYS:HA	1:A:28:ALA:H	1	0.01	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB1	1	0.01	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB2	1	0.01	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB3	1	0.01	0.01
(1,48)	1:A:16:ILE:HG12	1:B:39:ASN:H	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,48)	1:A:16:ILE:HG13	1:B:39:ASN:H	1	0.01	0.01
(1,476)	1:A:26:HIS:HB3	1:A:28:ALA:H	1	0.02	0.02
(1,460)	1:A:23:LEU:HD21	1:A:28:ALA:H	1	0.01	0.01
(1,460)	1:A:23:LEU:HD22	1:A:28:ALA:H	1	0.01	0.01
(1,460)	1:A:23:LEU:HD23	1:A:28:ALA:H	1	0.01	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB1	1	0.01	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB2	1	0.01	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB3	1	0.01	0.01
(1,438)	1:A:22:VAL:HG21	1:A:25:LYS:HD2	1	0.01	0.01
(1,438)	1:A:22:VAL:HG21	1:A:25:LYS:HD3	1	0.01	0.01
(1,438)	1:A:22:VAL:HG22	1:A:25:LYS:HD2	1	0.01	0.01
(1,438)	1:A:22:VAL:HG22	1:A:25:LYS:HD3	1	0.01	0.01
(1,438)	1:A:22:VAL:HG23	1:A:25:LYS:HD2	1	0.01	0.01
(1,438)	1:A:22:VAL:HG23	1:A:25:LYS:HD3	1	0.01	0.01
(1,428)	1:A:21:VAL:HG21	1:A:24:GLU:HB2	1	0.01	0.01
(1,428)	1:A:21:VAL:HG21	1:A:24:GLU:HB3	1	0.01	0.01
(1,428)	1:A:21:VAL:HG22	1:A:24:GLU:HB2	1	0.01	0.01
(1,428)	1:A:21:VAL:HG22	1:A:24:GLU:HB3	1	0.01	0.01
(1,428)	1:A:21:VAL:HG23	1:A:24:GLU:HB2	1	0.01	0.01
(1,428)	1:A:21:VAL:HG23	1:A:24:GLU:HB3	1	0.01	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD11	1	0.01	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD12	1	0.01	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD13	1	0.01	0.01
(1,39)	1:A:16:ILE:HA	1:B:36:ALA:HA	1	0.01	0.01
(1,386)	1:A:16:ILE:HA	1:A:19:ILE:HB	1	0.01	0.01
(1,37)	1:A:15:LEU:HD21	1:B:36:ALA:H	1	0.01	0.01
(1,37)	1:A:15:LEU:HD22	1:B:36:ALA:H	1	0.01	0.01
(1,37)	1:A:15:LEU:HD23	1:B:36:ALA:H	1	0.01	0.01
(1,361)	1:A:12:VAL:H	1:A:15:LEU:H	1	0.01	0.01
(1,337)	1:A:10:THR:HA	1:A:13:GLU:HB2	1	0.01	0.01
(1,337)	1:A:10:THR:HA	1:A:13:GLU:HB3	1	0.01	0.01
(1,326)	1:A:8:SER:H	1:A:11:GLN:HG2	1	0.01	0.01
(1,326)	1:A:8:SER:H	1:A:11:GLN:HG3	1	0.01	0.01
(1,32)	1:A:15:LEU:HD21	1:B:26:HIS:HB2	1	0.01	0.01
(1,32)	1:A:15:LEU:HD21	1:B:26:HIS:HB3	1	0.01	0.01
(1,32)	1:A:15:LEU:HD22	1:B:26:HIS:HB2	1	0.01	0.01
(1,32)	1:A:15:LEU:HD22	1:B:26:HIS:HB3	1	0.01	0.01
(1,32)	1:A:15:LEU:HD23	1:B:26:HIS:HB2	1	0.01	0.01
(1,32)	1:A:15:LEU:HD23	1:B:26:HIS:HB3	1	0.01	0.01
(1,310)	1:A:5:SER:HB2	1:A:7:TYR:H	1	0.01	0.01
(1,310)	1:A:5:SER:HB3	1:A:7:TYR:H	1	0.01	0.01
(1,309)	1:A:5:SER:HA	1:A:7:TYR:H	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD21	1	0.01	0.01
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD22	1	0.01	0.01
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD23	1	0.01	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD21	1	0.01	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD22	1	0.01	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD23	1	0.01	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD21	1	0.01	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD22	1	0.01	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD23	1	0.01	0.01
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG21	1	0.03	0.03
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG22	1	0.03	0.03
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG23	1	0.03	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG21	1	0.03	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG22	1	0.03	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG23	1	0.03	0.03
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD11	1	0.01	0.01
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD12	1	0.01	0.01
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD13	1	0.01	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD21	1	0.01	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD22	1	0.01	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD23	1	0.01	0.01
(1,261)	1:B:38:GLY:HA2	1:A:65:LEU:HB2	1	0.01	0.01
(1,261)	1:B:38:GLY:HA2	1:A:65:LEU:HB3	1	0.01	0.01
(1,261)	1:B:38:GLY:HA3	1:A:65:LEU:HB2	1	0.01	0.01
(1,261)	1:B:38:GLY:HA3	1:A:65:LEU:HB3	1	0.01	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD11	1	0.01	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD12	1	0.01	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD13	1	0.01	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD21	1	0.01	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD22	1	0.01	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD23	1	0.01	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD11	1	0.01	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD12	1	0.01	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD13	1	0.01	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD11	1	0.01	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD12	1	0.01	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD13	1	0.01	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD11	1	0.01	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD12	1	0.01	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD13	1	0.01	0.01
(1,230)	1:B:20:LEU:HD21	1:A:43:HIS:HB2	1	0.02	0.02
(1,230)	1:B:20:LEU:HD21	1:A:43:HIS:HB3	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,230)	1:B:20:LEU:HD22	1:A:43:HIS:HB2	1	0.02	0.02
(1,230)	1:B:20:LEU:HD22	1:A:43:HIS:HB3	1	0.02	0.02
(1,230)	1:B:20:LEU:HD23	1:A:43:HIS:HB2	1	0.02	0.02
(1,230)	1:B:20:LEU:HD23	1:A:43:HIS:HB3	1	0.02	0.02
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE1	1	0.01	0.01
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE2	1	0.01	0.01
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE3	1	0.01	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE1	1	0.01	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE2	1	0.01	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE3	1	0.01	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE1	1	0.01	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE2	1	0.01	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE3	1	0.01	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD11	1	0.01	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD12	1	0.01	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD13	1	0.01	0.01
(1,191)	1:B:15:LEU:HD21	1:A:36:ALA:H	1	0.01	0.01
(1,191)	1:B:15:LEU:HD22	1:A:36:ALA:H	1	0.01	0.01
(1,191)	1:B:15:LEU:HD23	1:A:36:ALA:H	1	0.01	0.01
(1,187)	1:B:15:LEU:HD21	1:A:26:HIS:HD2	1	0.01	0.01
(1,187)	1:B:15:LEU:HD22	1:A:26:HIS:HD2	1	0.01	0.01
(1,187)	1:B:15:LEU:HD23	1:A:26:HIS:HD2	1	0.01	0.01
(1,186)	1:B:15:LEU:HD21	1:A:26:HIS:HB2	1	0.02	0.02
(1,186)	1:B:15:LEU:HD21	1:A:26:HIS:HB3	1	0.02	0.02
(1,186)	1:B:15:LEU:HD22	1:A:26:HIS:HB2	1	0.02	0.02
(1,186)	1:B:15:LEU:HD22	1:A:26:HIS:HB3	1	0.02	0.02
(1,186)	1:B:15:LEU:HD23	1:A:26:HIS:HB2	1	0.02	0.02
(1,186)	1:B:15:LEU:HD23	1:A:26:HIS:HB3	1	0.02	0.02
(1,183)	1:B:15:LEU:HD11	1:A:26:HIS:HD2	1	0.01	0.01
(1,183)	1:B:15:LEU:HD12	1:A:26:HIS:HD2	1	0.01	0.01
(1,183)	1:B:15:LEU:HD13	1:A:26:HIS:HD2	1	0.01	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD21	1	0.01	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD22	1	0.01	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD23	1	0.01	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD21	1	0.01	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD22	1	0.01	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD23	1	0.01	0.01
(1,1475)	1:B:65:LEU:H	1:B:61:PHE:O	1	0.01	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD21	1	0.01	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD22	1	0.01	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD23	1	0.01	0.01
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD21	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD22	1	0.01	0.01
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD23	1	0.01	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD21	1	0.01	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD22	1	0.01	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD23	1	0.01	0.01
(1,1461)	1:B:58:ALA:H	1:B:54:ARG:O	1	0.01	0.01
(1,1457)	1:B:40:CYS:H	1:B:36:ALA:O	1	0.01	0.01
(1,1449)	1:B:35:MET:H	1:B:31:ASP:O	1	0.01	0.01
(1,1441)	1:B:22:VAL:H	1:B:18:GLU:O	1	0.01	0.01
(1,1415)	1:A:66:ALA:H	1:A:62:ALA:O	1	0.01	0.01
(1,1409)	1:A:63:LYS:H	1:A:59:GLU:O	1	0.01	0.01
(1,1401)	1:A:59:GLU:H	1:A:55:GLN:O	1	0.01	0.01
(1,1386)	1:A:24:GLU:N	1:A:20:LEU:O	1	0.01	0.01
(1,1373)	1:A:18:GLU:H	1:A:14:SER:O	1	0.01	0.01
(1,1367)	1:A:15:LEU:H	1:A:11:GLN:O	1	0.01	0.01
(1,1364)	1:A:13:GLU:N	1:A:9:ASN:O	1	0.01	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD11	1	0.01	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD12	1	0.01	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD13	1	0.01	0.01
(1,1349)	1:B:68:SER:HA	1:B:70:LYS:H	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG21	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG22	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG23	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG21	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG22	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG23	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG21	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG22	1	0.01	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG23	1	0.01	0.01
(1,1300)	1:B:60:GLN:HB2	1:B:62:ALA:H	1	0.01	0.01
(1,1300)	1:B:60:GLN:HB3	1:B:62:ALA:H	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB1	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB2	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB3	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB1	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB2	1	0.01	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB3	1	0.01	0.01
(1,127)	1:A:42:THR:HG21	1:B:68:SER:H	1	0.01	0.01
(1,127)	1:A:42:THR:HG22	1:B:68:SER:H	1	0.01	0.01
(1,127)	1:A:42:THR:HG23	1:B:68:SER:H	1	0.01	0.01
(1,1264)	1:B:56:ALA:HB1	1:B:59:GLU:HB2	1	0.01	0.01
(1,1264)	1:B:56:ALA:HB1	1:B:59:GLU:HB3	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1264)	1:B:56:ALA:HB2	1:B:59:GLU:HB2	1	0.01	0.01
(1,1264)	1:B:56:ALA:HB2	1:B:59:GLU:HB3	1	0.01	0.01
(1,1264)	1:B:56:ALA:HB3	1:B:59:GLU:HB2	1	0.01	0.01
(1,1264)	1:B:56:ALA:HB3	1:B:59:GLU:HB3	1	0.01	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD11	1	0.01	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD12	1	0.01	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD13	1	0.01	0.01
(1,1188)	1:B:47:ARG:HA	1:B:49:VAL:H	1	0.01	0.01
(1,1185)	1:B:46:GLU:HG2	1:B:54:ARG:HE	1	0.01	0.01
(1,1185)	1:B:46:GLU:HG3	1:B:54:ARG:HE	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD21	1:B:54:ARG:HD2	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD21	1:B:54:ARG:HD3	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD22	1:B:54:ARG:HD2	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD22	1:B:54:ARG:HD3	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD23	1:B:54:ARG:HD2	1	0.01	0.01
(1,1172)	1:B:45:LEU:HD23	1:B:54:ARG:HD3	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG11	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG12	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG13	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG11	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG12	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG13	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG11	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG12	1	0.01	0.01
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG13	1	0.01	0.01
(1,1152)	1:B:43:HIS:HD2	1:B:44:LEU:HA	1	0.01	0.01
(1,1148)	1:B:42:THR:HG21	1:B:46:GLU:H	1	0.01	0.01
(1,1148)	1:B:42:THR:HG22	1:B:46:GLU:H	1	0.01	0.01
(1,1148)	1:B:42:THR:HG23	1:B:46:GLU:H	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG11	1:B:45:LEU:HB2	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG11	1:B:45:LEU:HB3	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG12	1:B:45:LEU:HB2	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG12	1:B:45:LEU:HB3	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG13	1:B:45:LEU:HB2	1	0.01	0.01
(1,1129)	1:B:41:VAL:HG13	1:B:45:LEU:HB3	1	0.01	0.01
(1,1083)	1:B:36:ALA:HB1	1:B:39:ASN:HB2	1	0.03	0.03
(1,1083)	1:B:36:ALA:HB1	1:B:39:ASN:HB3	1	0.03	0.03
(1,1083)	1:B:36:ALA:HB2	1:B:39:ASN:HB2	1	0.03	0.03
(1,1083)	1:B:36:ALA:HB2	1:B:39:ASN:HB3	1	0.03	0.03
(1,1083)	1:B:36:ALA:HB3	1:B:39:ASN:HB2	1	0.03	0.03
(1,1083)	1:B:36:ALA:HB3	1:B:39:ASN:HB3	1	0.03	0.03
(1,1077)	1:B:35:MET:HB2	1:B:39:ASN:HD21	1	0.01	0.01

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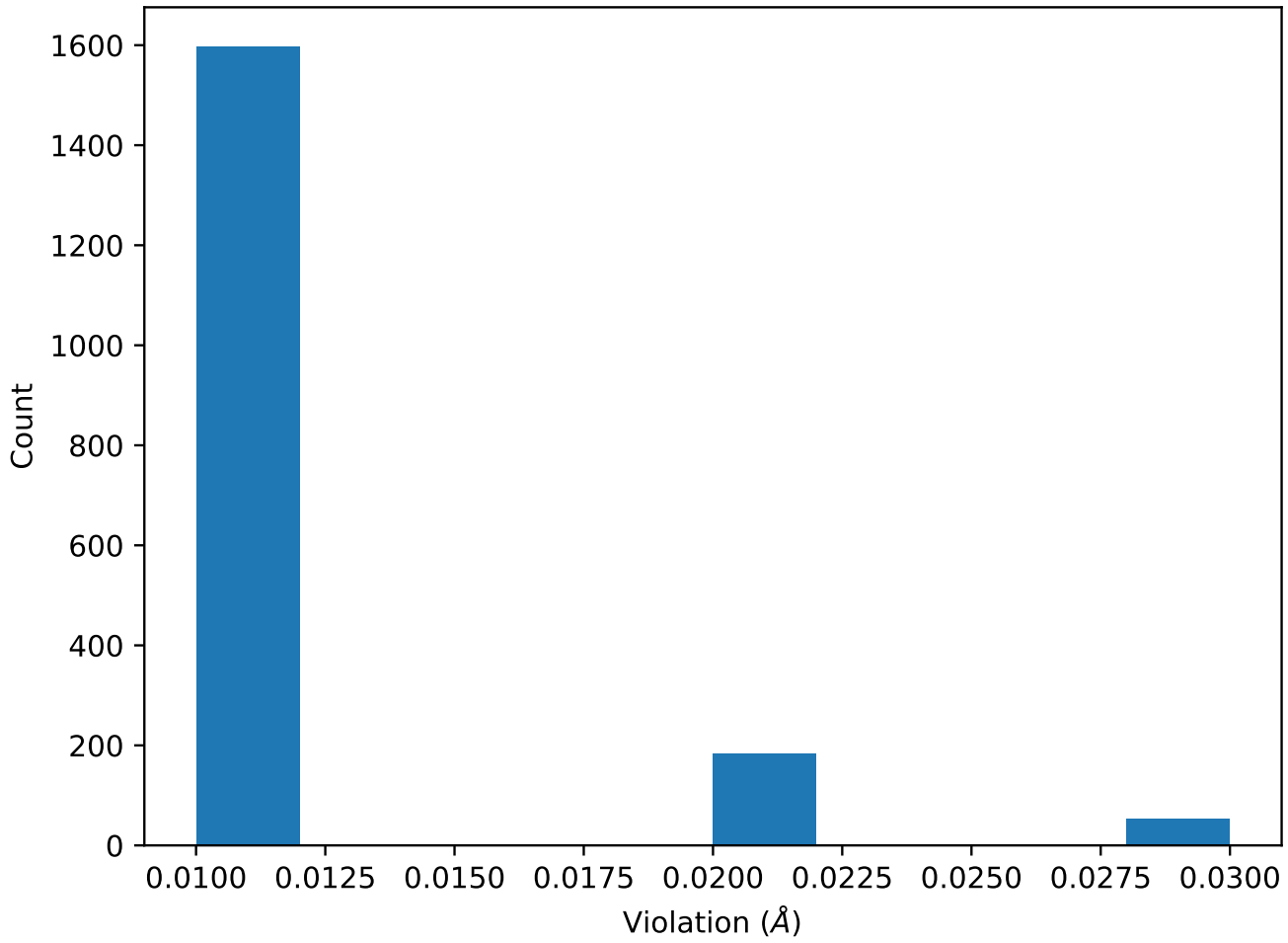
Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1077)	1:B:35:MET:HB2	1:B:39:ASN:HD22	1	0.01	0.01
(1,1077)	1:B:35:MET:HB3	1:B:39:ASN:HD21	1	0.01	0.01
(1,1077)	1:B:35:MET:HB3	1:B:39:ASN:HD22	1	0.01	0.01
(1,100)	1:A:37:LEU:HD11	1:B:41:VAL:HB	1	0.02	0.02
(1,100)	1:A:37:LEU:HD12	1:B:41:VAL:HB	1	0.02	0.02
(1,100)	1:A:37:LEU:HD13	1:B:41:VAL:HB	1	0.02	0.02

8.8 All distance violations

8.8.1 Histogram : Distribution of distance violations

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



8.8.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE1	13	0.03
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE2	13	0.03
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE1	13	0.03
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE2	13	0.03
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB1	10	0.03
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB2	10	0.03
(1,747)	1:A:57:VAL:HG11	1:A:58:ALA:HB3	10	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB1	10	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB2	10	0.03
(1,747)	1:A:57:VAL:HG12	1:A:58:ALA:HB3	10	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB1	10	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB2	10	0.03
(1,747)	1:A:57:VAL:HG13	1:A:58:ALA:HB3	10	0.03
(1,561)	1:A:37:LEU:HB2	1:A:41:VAL:H	17	0.03
(1,561)	1:A:37:LEU:HB3	1:A:41:VAL:H	17	0.03
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD1	8	0.03
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD2	8	0.03
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD1	8	0.03
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD2	8	0.03
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG21	6	0.03
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG22	6	0.03
(1,298)	1:B:55:GLN:HG2	1:A:69:VAL:HG23	6	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG21	6	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG22	6	0.03
(1,298)	1:B:55:GLN:HG3	1:A:69:VAL:HG23	6	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB1	3	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB2	3	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB3	3	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB1	3	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB2	3	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB3	3	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB1	3	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB2	3	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB3	3	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB1	9	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB2	9	0.03
(1,1274)	1:B:57:VAL:HG11	1:B:58:ALA:HB3	9	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB1	9	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB2	9	0.03
(1,1274)	1:B:57:VAL:HG12	1:B:58:ALA:HB3	9	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB1	9	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB2	9	0.03
(1,1274)	1:B:57:VAL:HG13	1:B:58:ALA:HB3	9	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	17	0.03
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	17	0.03
(1,1083)	1:B:36:ALA:HB1	1:B:39:ASN:HB2	4	0.03
(1,1083)	1:B:36:ALA:HB1	1:B:39:ASN:HB3	4	0.03
(1,1083)	1:B:36:ALA:HB2	1:B:39:ASN:HB2	4	0.03
(1,1083)	1:B:36:ALA:HB2	1:B:39:ASN:HB3	4	0.03
(1,1083)	1:B:36:ALA:HB3	1:B:39:ASN:HB2	4	0.03
(1,1083)	1:B:36:ALA:HB3	1:B:39:ASN:HB3	4	0.03
(1,1003)	1:B:26:HIS:HB3	1:B:28:ALA:H	15	0.03
(1,971)	1:B:23:LEU:HA	1:B:26:HIS:HD2	16	0.02
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG21	20	0.02
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG22	20	0.02
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG23	20	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG21	20	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG22	20	0.02
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG23	20	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG21	20	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG22	20	0.02
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG23	20	0.02
(1,836)	1:B:5:SER:HA	1:B:7:TYR:H	7	0.02
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD11	7	0.02
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD12	7	0.02
(1,78)	1:A:20:LEU:HD21	1:B:44:LEU:HD13	7	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD11	7	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD12	7	0.02
(1,78)	1:A:20:LEU:HD22	1:B:44:LEU:HD13	7	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD11	7	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD12	7	0.02
(1,78)	1:A:20:LEU:HD23	1:B:44:LEU:HD13	7	0.02
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD2	10	0.02
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD3	10	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	2	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	2	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	2	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	3	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	3	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	3	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	9	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	9	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	9	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	10	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	10	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	10	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	17	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	17	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	17	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	18	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	18	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	18	0.02
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	19	0.02
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	19	0.02
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	19	0.02
(1,696)	1:A:51:SER:HB2	1:A:53:SER:H	15	0.02
(1,696)	1:A:51:SER:HB3	1:A:53:SER:H	15	0.02
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	10	0.02
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	13	0.02
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	18	0.02
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	18	0.02
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	18	0.02
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	18	0.02
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	1	0.02
(1,589)	1:A:40:CYS:HB2	1:A:43:HIS:HB2	10	0.02
(1,589)	1:A:40:CYS:HB2	1:A:43:HIS:HB3	10	0.02
(1,589)	1:A:40:CYS:HB3	1:A:43:HIS:HB2	10	0.02
(1,589)	1:A:40:CYS:HB3	1:A:43:HIS:HB3	10	0.02
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	11	0.02
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	16	0.02
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	10	0.02
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	10	0.02
(1,561)	1:A:37:LEU:HB2	1:A:41:VAL:H	12	0.02
(1,561)	1:A:37:LEU:HB3	1:A:41:VAL:H	12	0.02
(1,476)	1:A:26:HIS:HB3	1:A:28:ALA:H	1	0.02
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE1	10	0.02
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE2	10	0.02
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE1	10	0.02
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE2	10	0.02
(1,280)	1:B:42:THR:HG21	1:A:65:LEU:HG	7	0.02
(1,280)	1:B:42:THR:HG22	1:A:65:LEU:HG	7	0.02
(1,280)	1:B:42:THR:HG23	1:A:65:LEU:HG	7	0.02
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	8	0.02
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	8	0.02
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	8	0.02
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	8	0.02
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	8	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	8	0.02
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	17	0.02
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	17	0.02
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	17	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	17	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	17	0.02
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	17	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	17	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	17	0.02
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	17	0.02
(1,230)	1:B:20:LEU:HD21	1:A:43:HIS:HB2	10	0.02
(1,230)	1:B:20:LEU:HD21	1:A:43:HIS:HB3	10	0.02
(1,230)	1:B:20:LEU:HD22	1:A:43:HIS:HB2	10	0.02
(1,230)	1:B:20:LEU:HD22	1:A:43:HIS:HB3	10	0.02
(1,230)	1:B:20:LEU:HD23	1:A:43:HIS:HB2	10	0.02
(1,230)	1:B:20:LEU:HD23	1:A:43:HIS:HB3	10	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	2	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	2	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	2	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	4	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	4	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	4	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	8	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	8	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	8	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	9	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	9	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	9	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	10	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	10	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	10	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	12	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	12	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	12	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	13	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	13	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	13	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	14	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	14	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	14	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	15	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	15	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	15	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	18	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	18	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	18	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	19	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	19	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	19	0.02
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	20	0.02
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	20	0.02
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	20	0.02
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG11	5	0.02
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG12	5	0.02
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG13	5	0.02
(1,186)	1:B:15:LEU:HD21	1:A:26:HIS:HB2	5	0.02
(1,186)	1:B:15:LEU:HD21	1:A:26:HIS:HB3	5	0.02
(1,186)	1:B:15:LEU:HD22	1:A:26:HIS:HB2	5	0.02
(1,186)	1:B:15:LEU:HD22	1:A:26:HIS:HB3	5	0.02
(1,186)	1:B:15:LEU:HD23	1:A:26:HIS:HB2	5	0.02
(1,186)	1:B:15:LEU:HD23	1:A:26:HIS:HB3	5	0.02
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE1	12	0.02
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE2	12	0.02
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE3	12	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE1	12	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE2	12	0.02
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE3	12	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE1	12	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE2	12	0.02
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE3	12	0.02
(1,1443)	1:B:23:LEU:H	1:B:19:ILE:O	18	0.02
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	12	0.02
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	12	0.02
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	12	0.02
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	12	0.02
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	12	0.02
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	12	0.02
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	13	0.02
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	16	0.02
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	16	0.02
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD2	14	0.02
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD3	14	0.02
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG2	20	0.02
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG3	20	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG2	20	0.02
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG3	20	0.02
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG2	20	0.02
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG3	20	0.02
(1,126)	1:A:42:THR:HG21	1:B:65:LEU:HG	2	0.02
(1,126)	1:A:42:THR:HG22	1:B:65:LEU:HG	2	0.02
(1,126)	1:A:42:THR:HG23	1:B:65:LEU:HG	2	0.02
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	7	0.02
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG2	10	0.02
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG3	10	0.02
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG2	10	0.02
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG3	10	0.02
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD21	17	0.02
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD22	17	0.02
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD23	17	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD21	17	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD22	17	0.02
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD23	17	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD21	17	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD22	17	0.02
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD23	17	0.02
(1,1003)	1:B:26:HIS:HB3	1:B:28:ALA:H	18	0.02
(1,100)	1:A:37:LEU:HD11	1:B:41:VAL:HB	17	0.02
(1,100)	1:A:37:LEU:HD12	1:B:41:VAL:HB	17	0.02
(1,100)	1:A:37:LEU:HD13	1:B:41:VAL:HB	17	0.02
(1,995)	1:B:24:GLU:HB2	1:B:26:HIS:H	20	0.01
(1,995)	1:B:24:GLU:HB3	1:B:26:HIS:H	20	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB1	7	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB2	7	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB3	7	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB1	13	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB2	13	0.01
(1,976)	1:B:23:LEU:HB2	1:B:28:ALA:HB3	13	0.01
(1,973)	1:B:23:LEU:HA	1:B:27:LYS:H	2	0.01
(1,973)	1:B:23:LEU:HA	1:B:27:LYS:H	9	0.01
(1,973)	1:B:23:LEU:HA	1:B:27:LYS:H	18	0.01
(1,971)	1:B:23:LEU:HA	1:B:26:HIS:HD2	4	0.01
(1,971)	1:B:23:LEU:HA	1:B:26:HIS:HD2	7	0.01
(1,971)	1:B:23:LEU:HA	1:B:26:HIS:HD2	13	0.01
(1,966)	1:B:22:VAL:HG21	1:B:25:LYS:HE2	17	0.01
(1,966)	1:B:22:VAL:HG21	1:B:25:LYS:HE3	17	0.01
(1,966)	1:B:22:VAL:HG22	1:B:25:LYS:HE2	17	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,966)	1:B:22:VAL:HG22	1:B:25:LYS:HE3	17	0.01
(1,966)	1:B:22:VAL:HG23	1:B:25:LYS:HE2	17	0.01
(1,966)	1:B:22:VAL:HG23	1:B:25:LYS:HE3	17	0.01
(1,963)	1:B:22:VAL:HG11	1:B:25:LYS:HB2	15	0.01
(1,963)	1:B:22:VAL:HG11	1:B:25:LYS:HB3	15	0.01
(1,963)	1:B:22:VAL:HG12	1:B:25:LYS:HB2	15	0.01
(1,963)	1:B:22:VAL:HG12	1:B:25:LYS:HB3	15	0.01
(1,963)	1:B:22:VAL:HG13	1:B:25:LYS:HB2	15	0.01
(1,963)	1:B:22:VAL:HG13	1:B:25:LYS:HB3	15	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE2	1	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE3	1	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE2	1	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE3	1	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE2	1	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE3	1	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE2	13	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE3	13	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE2	13	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE3	13	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE2	13	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE3	13	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE2	15	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE3	15	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE2	15	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE3	15	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE2	15	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE3	15	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE2	17	0.01
(1,953)	1:B:21:VAL:HG11	1:B:25:LYS:HE3	17	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE2	17	0.01
(1,953)	1:B:21:VAL:HG12	1:B:25:LYS:HE3	17	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE2	17	0.01
(1,953)	1:B:21:VAL:HG13	1:B:25:LYS:HE3	17	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG21	10	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG22	10	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG23	10	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG21	10	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG22	10	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG23	10	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG21	10	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG22	10	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG23	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG21	12	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG22	12	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG23	12	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG21	12	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG22	12	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG23	12	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG21	12	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG22	12	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG23	12	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG21	13	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG22	13	0.01
(1,95)	1:A:34:LEU:HD21	1:B:57:VAL:HG23	13	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG21	13	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG22	13	0.01
(1,95)	1:A:34:LEU:HD22	1:B:57:VAL:HG23	13	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG21	13	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG22	13	0.01
(1,95)	1:A:34:LEU:HD23	1:B:57:VAL:HG23	13	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	2	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	2	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	2	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	3	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	3	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	3	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	7	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	7	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	7	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	9	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	9	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	9	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	13	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	13	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	13	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	16	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	16	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	16	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD11	18	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD12	18	0.01
(1,931)	1:B:18:GLU:H	1:B:19:ILE:HD13	18	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG21	1	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG22	1	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG23	1	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG21	1	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG22	1	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG23	1	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG21	3	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG22	3	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG23	3	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG21	3	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG22	3	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG23	3	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG21	9	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG22	9	0.01
(1,894)	1:B:13:GLU:HG2	1:B:16:ILE:HG23	9	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG21	9	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG22	9	0.01
(1,894)	1:B:13:GLU:HG3	1:B:16:ILE:HG23	9	0.01
(1,89)	1:A:34:LEU:HA	1:B:41:VAL:HA	6	0.01
(1,89)	1:A:34:LEU:HA	1:B:41:VAL:HA	8	0.01
(1,89)	1:A:34:LEU:HA	1:B:41:VAL:HA	12	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD11	5	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD12	5	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD13	5	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD11	11	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD12	11	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD13	11	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD11	16	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD12	16	0.01
(1,877)	1:B:12:VAL:HA	1:B:15:LEU:HD13	16	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	8	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	8	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	8	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	8	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	8	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	8	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	10	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	10	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	10	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	10	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	10	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	10	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG21	14	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG22	14	0.01
(1,847)	1:B:7:TYR:HE1	1:B:12:VAL:HG23	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG21	14	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG22	14	0.01
(1,847)	1:B:7:TYR:HE2	1:B:12:VAL:HG23	14	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB2	10	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB3	10	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB2	10	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB3	10	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB2	13	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB3	13	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB2	13	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB3	13	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB2	17	0.01
(1,845)	1:B:7:TYR:HD1	1:B:11:GLN:HB3	17	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB2	17	0.01
(1,845)	1:B:7:TYR:HD2	1:B:11:GLN:HB3	17	0.01
(1,840)	1:B:6:LYS:HD2	1:B:7:TYR:HD1	9	0.01
(1,840)	1:B:6:LYS:HD2	1:B:7:TYR:HD2	9	0.01
(1,840)	1:B:6:LYS:HD3	1:B:7:TYR:HD1	9	0.01
(1,840)	1:B:6:LYS:HD3	1:B:7:TYR:HD2	9	0.01
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE1	3	0.01
(1,839)	1:B:6:LYS:HB2	1:B:7:TYR:HE2	3	0.01
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE1	3	0.01
(1,839)	1:B:6:LYS:HB3	1:B:7:TYR:HE2	3	0.01
(1,836)	1:B:5:SER:HA	1:B:7:TYR:H	17	0.01
(1,835)	1:A:72:ASN:H	1:A:73:LEU:HB2	10	0.01
(1,835)	1:A:72:ASN:H	1:A:73:LEU:HB3	10	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD11	14	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD12	14	0.01
(1,832)	1:A:70:LYS:HA	1:A:73:LEU:HD13	14	0.01
(1,83)	1:A:30:THR:HG21	1:B:48:LYS:HA	12	0.01
(1,83)	1:A:30:THR:HG22	1:B:48:LYS:HA	12	0.01
(1,83)	1:A:30:THR:HG23	1:B:48:LYS:HA	12	0.01
(1,83)	1:A:30:THR:HG21	1:B:48:LYS:HA	16	0.01
(1,83)	1:A:30:THR:HG22	1:B:48:LYS:HA	16	0.01
(1,83)	1:A:30:THR:HG23	1:B:48:LYS:HA	16	0.01
(1,829)	1:A:69:VAL:H	1:A:70:LYS:HB2	10	0.01
(1,829)	1:A:69:VAL:H	1:A:70:LYS:HB3	10	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD21	14	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD22	14	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD21	16	0.01
(1,828)	1:A:69:VAL:HA	1:A:72:ASN:HD22	16	0.01
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD21	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD22	7	0.01
(1,82)	1:A:30:THR:HG21	1:B:44:LEU:HD23	7	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD21	7	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD22	7	0.01
(1,82)	1:A:30:THR:HG22	1:B:44:LEU:HD23	7	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD21	7	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD22	7	0.01
(1,82)	1:A:30:THR:HG23	1:B:44:LEU:HD23	7	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB2	7	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB3	7	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB2	7	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB3	7	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB2	7	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB3	7	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB2	15	0.01
(1,817)	1:A:66:ALA:HB1	1:A:70:LYS:HB3	15	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB2	15	0.01
(1,817)	1:A:66:ALA:HB2	1:A:70:LYS:HB3	15	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB2	15	0.01
(1,817)	1:A:66:ALA:HB3	1:A:70:LYS:HB3	15	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG21	5	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG22	5	0.01
(1,809)	1:A:65:LEU:HD11	1:A:69:VAL:HG23	5	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG21	5	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG22	5	0.01
(1,809)	1:A:65:LEU:HD12	1:A:69:VAL:HG23	5	0.01
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG21	5	0.01
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG22	5	0.01
(1,809)	1:A:65:LEU:HD13	1:A:69:VAL:HG23	5	0.01
(1,808)	1:A:65:LEU:HB2	1:A:68:SER:H	9	0.01
(1,808)	1:A:65:LEU:HB3	1:A:68:SER:H	9	0.01
(1,808)	1:A:65:LEU:HB2	1:A:68:SER:H	10	0.01
(1,808)	1:A:65:LEU:HB3	1:A:68:SER:H	10	0.01
(1,808)	1:A:65:LEU:HB2	1:A:68:SER:H	13	0.01
(1,808)	1:A:65:LEU:HB3	1:A:68:SER:H	13	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD21	7	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD22	7	0.01
(1,794)	1:A:62:ALA:HB1	1:A:65:LEU:HD23	7	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD21	7	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD22	7	0.01
(1,794)	1:A:62:ALA:HB2	1:A:65:LEU:HD23	7	0.01
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD21	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD22	7	0.01
(1,794)	1:A:62:ALA:HB3	1:A:65:LEU:HD23	7	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB1	6	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB2	6	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB3	6	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB1	6	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB2	6	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB3	6	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB1	7	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB2	7	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB3	7	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB1	7	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB2	7	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB3	7	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB1	11	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB2	11	0.01
(1,782)	1:A:61:PHE:HE1	1:A:64:ALA:HB3	11	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB1	11	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB2	11	0.01
(1,782)	1:A:61:PHE:HE2	1:A:64:ALA:HB3	11	0.01
(1,780)	1:A:61:PHE:HD1	1:A:65:LEU:HB2	7	0.01
(1,780)	1:A:61:PHE:HD1	1:A:65:LEU:HB3	7	0.01
(1,780)	1:A:61:PHE:HD2	1:A:65:LEU:HB2	7	0.01
(1,780)	1:A:61:PHE:HD2	1:A:65:LEU:HB3	7	0.01
(1,774)	1:A:60:GLN:HB2	1:A:63:LYS:H	18	0.01
(1,774)	1:A:60:GLN:HB3	1:A:63:LYS:H	18	0.01
(1,773)	1:A:60:GLN:HB2	1:A:62:ALA:H	1	0.01
(1,773)	1:A:60:GLN:HB3	1:A:62:ALA:H	1	0.01
(1,773)	1:A:60:GLN:HB2	1:A:62:ALA:H	5	0.01
(1,773)	1:A:60:GLN:HB3	1:A:62:ALA:H	5	0.01
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD2	20	0.01
(1,770)	1:A:60:GLN:HA	1:A:63:LYS:HD3	20	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB1	12	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB2	12	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB3	12	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB1	12	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB2	12	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB3	12	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB1	20	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB2	20	0.01
(1,766)	1:A:59:GLU:HG2	1:A:62:ALA:HB3	20	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB1	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB2	20	0.01
(1,766)	1:A:59:GLU:HG3	1:A:62:ALA:HB3	20	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE2	11	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE3	11	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE2	11	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE3	11	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE2	16	0.01
(1,765)	1:A:59:GLU:HB2	1:A:63:LYS:HE3	16	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE2	16	0.01
(1,765)	1:A:59:GLU:HB3	1:A:63:LYS:HE3	16	0.01
(1,749)	1:A:57:VAL:HG11	1:A:61:PHE:H	10	0.01
(1,749)	1:A:57:VAL:HG12	1:A:61:PHE:H	10	0.01
(1,749)	1:A:57:VAL:HG13	1:A:61:PHE:H	10	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG2	3	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG3	3	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG2	3	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG3	3	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG2	3	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG3	3	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG2	4	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG3	4	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG2	4	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG3	4	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG2	4	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG3	4	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG2	17	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG3	17	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG2	17	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG3	17	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG2	17	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG3	17	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG2	19	0.01
(1,738)	1:A:56:ALA:HB1	1:A:59:GLU:HG3	19	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG2	19	0.01
(1,738)	1:A:56:ALA:HB2	1:A:59:GLU:HG3	19	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG2	19	0.01
(1,738)	1:A:56:ALA:HB3	1:A:59:GLU:HG3	19	0.01
(1,73)	1:A:20:LEU:HD11	1:B:43:HIS:HE1	5	0.01
(1,73)	1:A:20:LEU:HD12	1:B:43:HIS:HE1	5	0.01
(1,73)	1:A:20:LEU:HD13	1:B:43:HIS:HE1	5	0.01
(1,73)	1:A:20:LEU:HD11	1:B:43:HIS:HE1	7	0.01
(1,73)	1:A:20:LEU:HD12	1:B:43:HIS:HE1	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,73)	1:A:20:LEU:HD13	1:B:43:HIS:HE1	7	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD2	1	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD3	1	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD2	11	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD3	11	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD2	15	0.01
(1,702)	1:A:51:SER:H	1:A:54:ARG:HD3	15	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	5	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	5	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	5	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	6	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	6	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	6	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	11	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	11	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	11	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	12	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	12	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	12	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	13	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	13	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	13	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	14	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	14	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	14	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	15	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	15	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	15	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	16	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	16	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	16	0.01
(1,70)	1:A:19:ILE:HG21	1:B:23:LEU:H	20	0.01
(1,70)	1:A:19:ILE:HG22	1:B:23:LEU:H	20	0.01
(1,70)	1:A:19:ILE:HG23	1:B:23:LEU:H	20	0.01
(1,698)	1:A:51:SER:HB2	1:A:54:ARG:HE	1	0.01
(1,698)	1:A:51:SER:HB3	1:A:54:ARG:HE	1	0.01
(1,698)	1:A:51:SER:HB2	1:A:54:ARG:HE	6	0.01
(1,698)	1:A:51:SER:HB3	1:A:54:ARG:HE	6	0.01
(1,698)	1:A:51:SER:HB2	1:A:54:ARG:HE	7	0.01
(1,698)	1:A:51:SER:HB3	1:A:54:ARG:HE	7	0.01
(1,698)	1:A:51:SER:HB2	1:A:54:ARG:HE	14	0.01
(1,698)	1:A:51:SER:HB3	1:A:54:ARG:HE	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,696)	1:A:51:SER:HB2	1:A:53:SER:H	2	0.01
(1,696)	1:A:51:SER:HB3	1:A:53:SER:H	2	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	1	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	2	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	9	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	15	0.01
(1,662)	1:A:47:ARG:H	1:A:48:LYS:HA	19	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	6	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	6	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	6	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	6	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	7	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	7	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	7	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	7	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	8	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	8	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	8	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	8	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG2	11	0.01
(1,659)	1:A:46:GLU:HG2	1:A:54:ARG:HG3	11	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG2	11	0.01
(1,659)	1:A:46:GLU:HG3	1:A:54:ARG:HG3	11	0.01
(1,658)	1:A:46:GLU:HG2	1:A:54:ARG:HE	2	0.01
(1,658)	1:A:46:GLU:HG3	1:A:54:ARG:HE	2	0.01
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	2	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	2	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	2	0.01
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	3	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	3	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	3	0.01
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	9	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	9	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	9	0.01
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	17	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	17	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	17	0.01
(1,65)	1:A:19:ILE:HD11	1:B:37:LEU:H	19	0.01
(1,65)	1:A:19:ILE:HD12	1:B:37:LEU:H	19	0.01
(1,65)	1:A:19:ILE:HD13	1:B:37:LEU:H	19	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	2	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	2	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	8	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	8	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	8	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	14	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	14	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	14	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	16	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	16	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	16	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	17	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	17	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	17	0.01
(1,647)	1:A:45:LEU:HD21	1:A:54:ARG:H	20	0.01
(1,647)	1:A:45:LEU:HD22	1:A:54:ARG:H	20	0.01
(1,647)	1:A:45:LEU:HD23	1:A:54:ARG:H	20	0.01
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD2	6	0.01
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD3	6	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD2	6	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD3	6	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD2	6	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD3	6	0.01
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD2	18	0.01
(1,645)	1:A:45:LEU:HD21	1:A:54:ARG:HD3	18	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD2	18	0.01
(1,645)	1:A:45:LEU:HD22	1:A:54:ARG:HD3	18	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD2	18	0.01
(1,645)	1:A:45:LEU:HD23	1:A:54:ARG:HD3	18	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	10	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	11	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	16	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	17	0.01
(1,626)	1:A:43:HIS:HD2	1:A:44:LEU:HG	20	0.01
(1,623)	1:A:43:HIS:HA	1:A:47:ARG:H	19	0.01
(1,621)	1:A:42:THR:HG21	1:A:46:GLU:H	3	0.01
(1,621)	1:A:42:THR:HG22	1:A:46:GLU:H	3	0.01
(1,621)	1:A:42:THR:HG23	1:A:46:GLU:H	3	0.01
(1,619)	1:A:42:THR:HA	1:A:46:GLU:H	19	0.01
(1,616)	1:A:42:THR:HA	1:A:45:LEU:HB2	14	0.01
(1,616)	1:A:42:THR:HA	1:A:45:LEU:HB3	14	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	3	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	3	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	3	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	3	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	3	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	3	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	3	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	3	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	3	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	8	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	8	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	8	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	8	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	8	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	8	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	8	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	8	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	8	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	11	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	11	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	11	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	11	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	11	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	11	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	11	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	11	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	11	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	19	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	19	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	19	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	19	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	19	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	19	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	19	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	19	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	19	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD21	20	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD22	20	0.01
(1,611)	1:A:41:VAL:HG11	1:A:65:LEU:HD23	20	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD21	20	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD22	20	0.01
(1,611)	1:A:41:VAL:HG12	1:A:65:LEU:HD23	20	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD21	20	0.01
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD22	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,611)	1:A:41:VAL:HG13	1:A:65:LEU:HD23	20	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	3	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	3	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	3	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	3	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	3	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	3	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	3	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	3	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	3	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	4	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	4	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	4	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	4	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	4	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	4	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	4	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	4	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	4	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	5	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	5	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	5	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	5	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	5	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	5	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	5	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	5	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	5	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	9	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	9	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	9	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	9	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	9	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	9	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	9	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	9	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	9	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	10	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	10	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	10	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	10	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	10	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	10	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	10	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	10	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	16	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	16	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	16	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	16	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	16	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	16	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	16	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	16	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	16	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD11	19	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD12	19	0.01
(1,610)	1:A:41:VAL:HG11	1:A:65:LEU:HD13	19	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD11	19	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD12	19	0.01
(1,610)	1:A:41:VAL:HG12	1:A:65:LEU:HD13	19	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD11	19	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD12	19	0.01
(1,610)	1:A:41:VAL:HG13	1:A:65:LEU:HD13	19	0.01
(1,60)	1:A:19:ILE:HD11	1:B:22:VAL:HB	4	0.01
(1,60)	1:A:19:ILE:HD12	1:B:22:VAL:HB	4	0.01
(1,60)	1:A:19:ILE:HD13	1:B:22:VAL:HB	4	0.01
(1,599)	1:A:41:VAL:HA	1:A:45:LEU:H	14	0.01
(1,599)	1:A:41:VAL:HA	1:A:45:LEU:H	17	0.01
(1,595)	1:A:41:VAL:HA	1:A:44:LEU:HB2	10	0.01
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	1	0.01
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	5	0.01
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	17	0.01
(1,587)	1:A:40:CYS:HA	1:A:43:HIS:HD2	20	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	3	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	3	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	4	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	4	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	7	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	7	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	13	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	13	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	14	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	17	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	17	0.01
(1,580)	1:A:39:ASN:HB2	1:A:42:THR:H	20	0.01
(1,580)	1:A:39:ASN:HB3	1:A:42:THR:H	20	0.01
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG11	15	0.01
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG12	15	0.01
(1,58)	1:A:18:GLU:H	1:B:22:VAL:HG13	15	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG21	4	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG22	4	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG23	4	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG21	4	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG22	4	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG23	4	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG21	16	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG22	16	0.01
(1,57)	1:A:18:GLU:HG2	1:B:22:VAL:HG23	16	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG21	16	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG22	16	0.01
(1,57)	1:A:18:GLU:HG3	1:B:22:VAL:HG23	16	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG21	13	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG22	13	0.01
(1,566)	1:A:38:GLY:HA3	1:A:41:VAL:HG23	13	0.01
(1,562)	1:A:37:LEU:HD11	1:A:40:CYS:HB2	2	0.01
(1,562)	1:A:37:LEU:HD11	1:A:40:CYS:HB3	2	0.01
(1,562)	1:A:37:LEU:HD12	1:A:40:CYS:HB2	2	0.01
(1,562)	1:A:37:LEU:HD12	1:A:40:CYS:HB3	2	0.01
(1,562)	1:A:37:LEU:HD13	1:A:40:CYS:HB2	2	0.01
(1,562)	1:A:37:LEU:HD13	1:A:40:CYS:HB3	2	0.01
(1,550)	1:A:35:MET:HB2	1:A:39:ASN:HD21	4	0.01
(1,550)	1:A:35:MET:HB2	1:A:39:ASN:HD22	4	0.01
(1,550)	1:A:35:MET:HB3	1:A:39:ASN:HD21	4	0.01
(1,550)	1:A:35:MET:HB3	1:A:39:ASN:HD22	4	0.01
(1,547)	1:A:34:LEU:H	1:A:37:LEU:H	20	0.01
(1,546)	1:A:34:LEU:H	1:A:37:LEU:HB2	12	0.01
(1,546)	1:A:34:LEU:H	1:A:37:LEU:HB3	12	0.01
(1,53)	1:A:16:ILE:HG21	1:B:43:HIS:HD2	2	0.01
(1,53)	1:A:16:ILE:HG22	1:B:43:HIS:HD2	2	0.01
(1,53)	1:A:16:ILE:HG23	1:B:43:HIS:HD2	2	0.01
(1,53)	1:A:16:ILE:HG21	1:B:43:HIS:HD2	4	0.01
(1,53)	1:A:16:ILE:HG22	1:B:43:HIS:HD2	4	0.01
(1,53)	1:A:16:ILE:HG23	1:B:43:HIS:HD2	4	0.01
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE1	18	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE2	18	0.01
(1,517)	1:A:31:ASP:HB2	1:A:35:MET:HE3	18	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE1	18	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE2	18	0.01
(1,517)	1:A:31:ASP:HB3	1:A:35:MET:HE3	18	0.01
(1,482)	1:A:27:LYS:HA	1:A:28:ALA:H	5	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB1	7	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB2	7	0.01
(1,480)	1:A:26:HIS:H	1:A:28:ALA:HB3	7	0.01
(1,48)	1:A:16:ILE:HG12	1:B:39:ASN:H	4	0.01
(1,48)	1:A:16:ILE:HG13	1:B:39:ASN:H	4	0.01
(1,460)	1:A:23:LEU:HD21	1:A:28:ALA:H	5	0.01
(1,460)	1:A:23:LEU:HD22	1:A:28:ALA:H	5	0.01
(1,460)	1:A:23:LEU:HD23	1:A:28:ALA:H	5	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB1	14	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB2	14	0.01
(1,449)	1:A:23:LEU:HB2	1:A:28:ALA:HB3	14	0.01
(1,446)	1:A:23:LEU:HA	1:A:27:LYS:H	5	0.01
(1,446)	1:A:23:LEU:HA	1:A:27:LYS:H	6	0.01
(1,446)	1:A:23:LEU:HA	1:A:27:LYS:H	17	0.01
(1,444)	1:A:23:LEU:HA	1:A:26:HIS:HD2	14	0.01
(1,444)	1:A:23:LEU:HA	1:A:26:HIS:HD2	15	0.01
(1,438)	1:A:22:VAL:HG21	1:A:25:LYS:HD2	16	0.01
(1,438)	1:A:22:VAL:HG21	1:A:25:LYS:HD3	16	0.01
(1,438)	1:A:22:VAL:HG22	1:A:25:LYS:HD2	16	0.01
(1,438)	1:A:22:VAL:HG22	1:A:25:LYS:HD3	16	0.01
(1,438)	1:A:22:VAL:HG23	1:A:25:LYS:HD2	16	0.01
(1,438)	1:A:22:VAL:HG23	1:A:25:LYS:HD3	16	0.01
(1,428)	1:A:21:VAL:HG21	1:A:24:GLU:HB2	20	0.01
(1,428)	1:A:21:VAL:HG21	1:A:24:GLU:HB3	20	0.01
(1,428)	1:A:21:VAL:HG22	1:A:24:GLU:HB2	20	0.01
(1,428)	1:A:21:VAL:HG22	1:A:24:GLU:HB3	20	0.01
(1,428)	1:A:21:VAL:HG23	1:A:24:GLU:HB2	20	0.01
(1,428)	1:A:21:VAL:HG23	1:A:24:GLU:HB3	20	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	1	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	1	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	1	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	7	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	7	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	7	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	8	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	8	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	18	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	18	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	18	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD11	20	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD12	20	0.01
(1,404)	1:A:18:GLU:H	1:A:19:ILE:HD13	20	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD11	7	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD12	7	0.01
(1,396)	1:A:17:ALA:HA	1:A:20:LEU:HD13	7	0.01
(1,39)	1:A:16:ILE:HA	1:B:36:ALA:HA	4	0.01
(1,386)	1:A:16:ILE:HA	1:A:19:ILE:HB	4	0.01
(1,37)	1:A:15:LEU:HD21	1:B:36:ALA:H	13	0.01
(1,37)	1:A:15:LEU:HD22	1:B:36:ALA:H	13	0.01
(1,37)	1:A:15:LEU:HD23	1:B:36:ALA:H	13	0.01
(1,361)	1:A:12:VAL:H	1:A:15:LEU:H	7	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD11	1	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD12	1	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD13	1	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD11	5	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD12	5	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD13	5	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD11	8	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD12	8	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD13	8	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD11	9	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD12	9	0.01
(1,350)	1:A:12:VAL:HA	1:A:15:LEU:HD13	9	0.01
(1,340)	1:A:10:THR:HG21	1:A:14:SER:H	3	0.01
(1,340)	1:A:10:THR:HG22	1:A:14:SER:H	3	0.01
(1,340)	1:A:10:THR:HG23	1:A:14:SER:H	3	0.01
(1,340)	1:A:10:THR:HG21	1:A:14:SER:H	18	0.01
(1,340)	1:A:10:THR:HG22	1:A:14:SER:H	18	0.01
(1,340)	1:A:10:THR:HG23	1:A:14:SER:H	18	0.01
(1,337)	1:A:10:THR:HA	1:A:13:GLU:HB2	7	0.01
(1,337)	1:A:10:THR:HA	1:A:13:GLU:HB3	7	0.01
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	7	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	7	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	7	0.01
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	9	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	9	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	13	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	13	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	13	0.01
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	14	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	14	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	14	0.01
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	15	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	15	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	15	0.01
(1,33)	1:A:15:LEU:HD21	1:B:26:HIS:HD2	16	0.01
(1,33)	1:A:15:LEU:HD22	1:B:26:HIS:HD2	16	0.01
(1,33)	1:A:15:LEU:HD23	1:B:26:HIS:HD2	16	0.01
(1,326)	1:A:8:SER:H	1:A:11:GLN:HG2	8	0.01
(1,326)	1:A:8:SER:H	1:A:11:GLN:HG3	8	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	9	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	9	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	9	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	9	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	9	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	9	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	12	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	12	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	12	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	12	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	12	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	12	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG21	19	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG22	19	0.01
(1,320)	1:A:7:TYR:HE1	1:A:12:VAL:HG23	19	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG21	19	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG22	19	0.01
(1,320)	1:A:7:TYR:HE2	1:A:12:VAL:HG23	19	0.01
(1,32)	1:A:15:LEU:HD21	1:B:26:HIS:HB2	18	0.01
(1,32)	1:A:15:LEU:HD21	1:B:26:HIS:HB3	18	0.01
(1,32)	1:A:15:LEU:HD22	1:B:26:HIS:HB2	18	0.01
(1,32)	1:A:15:LEU:HD22	1:B:26:HIS:HB3	18	0.01
(1,32)	1:A:15:LEU:HD23	1:B:26:HIS:HB2	18	0.01
(1,32)	1:A:15:LEU:HD23	1:B:26:HIS:HB3	18	0.01
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD1	1	0.01
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD2	1	0.01
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD1	1	0.01
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD2	1	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD1	10	0.01
(1,314)	1:A:6:LYS:HE2	1:A:7:TYR:HD2	10	0.01
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD1	10	0.01
(1,314)	1:A:6:LYS:HE3	1:A:7:TYR:HD2	10	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD1	3	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD2	3	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD1	3	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD2	3	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD1	7	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD2	7	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD1	7	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD2	7	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD1	9	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD2	9	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD1	9	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD2	9	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD1	19	0.01
(1,313)	1:A:6:LYS:HD2	1:A:7:TYR:HD2	19	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD1	19	0.01
(1,313)	1:A:6:LYS:HD3	1:A:7:TYR:HD2	19	0.01
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE1	20	0.01
(1,312)	1:A:6:LYS:HB2	1:A:7:TYR:HE2	20	0.01
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE1	20	0.01
(1,312)	1:A:6:LYS:HB3	1:A:7:TYR:HE2	20	0.01
(1,310)	1:A:5:SER:HB2	1:A:7:TYR:H	12	0.01
(1,310)	1:A:5:SER:HB3	1:A:7:TYR:H	12	0.01
(1,309)	1:A:5:SER:HA	1:A:7:TYR:H	2	0.01
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD21	20	0.01
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD22	20	0.01
(1,307)	1:B:62:ALA:HB1	1:A:65:LEU:HD23	20	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD21	20	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD22	20	0.01
(1,307)	1:B:62:ALA:HB2	1:A:65:LEU:HD23	20	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD21	20	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD22	20	0.01
(1,307)	1:B:62:ALA:HB3	1:A:65:LEU:HD23	20	0.01
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG2	1	0.01
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG3	1	0.01
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG2	1	0.01
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG3	1	0.01
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG2	20	0.01
(1,299)	1:B:55:GLN:HG2	1:A:70:LYS:HG3	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG2	20	0.01
(1,299)	1:B:55:GLN:HG3	1:A:70:LYS:HG3	20	0.01
(1,280)	1:B:42:THR:HG21	1:A:65:LEU:HG	20	0.01
(1,280)	1:B:42:THR:HG22	1:A:65:LEU:HG	20	0.01
(1,280)	1:B:42:THR:HG23	1:A:65:LEU:HG	20	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	3	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	3	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	3	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	3	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	3	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	3	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	4	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	4	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	4	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	4	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	4	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	4	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	6	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	6	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	6	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	6	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	6	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	6	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	9	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	9	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	9	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	9	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	9	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	9	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	10	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	10	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	10	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	10	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	10	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	10	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	11	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	11	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	11	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	11	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	11	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	11	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	14	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	14	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	14	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	14	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	14	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	15	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	15	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	15	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	15	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	15	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	15	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	17	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	17	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	17	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	17	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	17	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	17	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	18	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	18	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	18	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	18	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	18	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	18	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB2	19	0.01
(1,278)	1:B:42:THR:HG21	1:A:65:LEU:HB3	19	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB2	19	0.01
(1,278)	1:B:42:THR:HG22	1:A:65:LEU:HB3	19	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB2	19	0.01
(1,278)	1:B:42:THR:HG23	1:A:65:LEU:HB3	19	0.01
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD11	20	0.01
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD12	20	0.01
(1,276)	1:B:42:THR:HB	1:A:65:LEU:HD13	20	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD21	12	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD22	12	0.01
(1,275)	1:B:42:THR:HA	1:A:65:LEU:HD23	12	0.01
(1,261)	1:B:38:GLY:HA2	1:A:65:LEU:HB2	20	0.01
(1,261)	1:B:38:GLY:HA2	1:A:65:LEU:HB3	20	0.01
(1,261)	1:B:38:GLY:HA3	1:A:65:LEU:HB2	20	0.01
(1,261)	1:B:38:GLY:HA3	1:A:65:LEU:HB3	20	0.01
(1,254)	1:B:37:LEU:HD11	1:A:41:VAL:HB	7	0.01
(1,254)	1:B:37:LEU:HD12	1:A:41:VAL:HB	7	0.01
(1,254)	1:B:37:LEU:HD13	1:A:41:VAL:HB	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,254)	1:B:37:LEU:HD11	1:A:41:VAL:HB	13	0.01
(1,254)	1:B:37:LEU:HD12	1:A:41:VAL:HB	13	0.01
(1,254)	1:B:37:LEU:HD13	1:A:41:VAL:HB	13	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	2	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	2	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	2	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	2	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	2	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	2	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	2	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	2	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	2	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	4	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	4	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	4	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	4	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	4	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	4	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	4	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	4	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	4	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	6	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	6	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	6	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	6	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	6	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	6	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	6	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	6	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	6	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	7	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	7	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	7	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	7	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	7	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	7	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	7	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	7	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	7	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG21	16	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG22	16	0.01
(1,249)	1:B:34:LEU:HD21	1:A:57:VAL:HG23	16	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG21	16	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG22	16	0.01
(1,249)	1:B:34:LEU:HD22	1:A:57:VAL:HG23	16	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG21	16	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG22	16	0.01
(1,249)	1:B:34:LEU:HD23	1:A:57:VAL:HG23	16	0.01
(1,243)	1:B:34:LEU:HA	1:A:41:VAL:HA	7	0.01
(1,243)	1:B:34:LEU:HA	1:A:41:VAL:HA	13	0.01
(1,243)	1:B:34:LEU:HA	1:A:41:VAL:HA	16	0.01
(1,243)	1:B:34:LEU:HA	1:A:41:VAL:HA	18	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD11	10	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD12	10	0.01
(1,240)	1:B:33:SER:HA	1:A:44:LEU:HD13	10	0.01
(1,237)	1:B:30:THR:HG21	1:A:48:LYS:HA	6	0.01
(1,237)	1:B:30:THR:HG22	1:A:48:LYS:HA	6	0.01
(1,237)	1:B:30:THR:HG23	1:A:48:LYS:HA	6	0.01
(1,237)	1:B:30:THR:HG21	1:A:48:LYS:HA	9	0.01
(1,237)	1:B:30:THR:HG22	1:A:48:LYS:HA	9	0.01
(1,237)	1:B:30:THR:HG23	1:A:48:LYS:HA	9	0.01
(1,237)	1:B:30:THR:HG21	1:A:48:LYS:HA	14	0.01
(1,237)	1:B:30:THR:HG22	1:A:48:LYS:HA	14	0.01
(1,237)	1:B:30:THR:HG23	1:A:48:LYS:HA	14	0.01
(1,237)	1:B:30:THR:HG21	1:A:48:LYS:HA	16	0.01
(1,237)	1:B:30:THR:HG22	1:A:48:LYS:HA	16	0.01
(1,237)	1:B:30:THR:HG23	1:A:48:LYS:HA	16	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD21	10	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD22	10	0.01
(1,235)	1:B:30:THR:HA	1:A:44:LEU:HD23	10	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD11	16	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD12	16	0.01
(1,232)	1:B:20:LEU:HD21	1:A:44:LEU:HD13	16	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD11	16	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD12	16	0.01
(1,232)	1:B:20:LEU:HD22	1:A:44:LEU:HD13	16	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD11	16	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD12	16	0.01
(1,232)	1:B:20:LEU:HD23	1:A:44:LEU:HD13	16	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	1	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	1	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	1	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	3	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	3	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	3	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	5	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	5	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	5	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	6	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	6	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	6	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	7	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	7	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	7	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	11	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	11	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	11	0.01
(1,224)	1:B:19:ILE:HG21	1:A:23:LEU:H	17	0.01
(1,224)	1:B:19:ILE:HG22	1:A:23:LEU:H	17	0.01
(1,224)	1:B:19:ILE:HG23	1:A:23:LEU:H	17	0.01
(1,219)	1:B:19:ILE:HD11	1:A:37:LEU:H	4	0.01
(1,219)	1:B:19:ILE:HD12	1:A:37:LEU:H	4	0.01
(1,219)	1:B:19:ILE:HD13	1:A:37:LEU:H	4	0.01
(1,219)	1:B:19:ILE:HD11	1:A:37:LEU:H	20	0.01
(1,219)	1:B:19:ILE:HD12	1:A:37:LEU:H	20	0.01
(1,219)	1:B:19:ILE:HD13	1:A:37:LEU:H	20	0.01
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG11	15	0.01
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG12	15	0.01
(1,212)	1:B:18:GLU:H	1:A:22:VAL:HG13	15	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG21	2	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG22	2	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG23	2	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG21	2	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG22	2	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG23	2	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG21	12	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG22	12	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG23	12	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG21	12	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG22	12	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG23	12	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG21	14	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG22	14	0.01
(1,211)	1:B:18:GLU:HG2	1:A:22:VAL:HG23	14	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG21	14	0.01
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG22	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,211)	1:B:18:GLU:HG3	1:A:22:VAL:HG23	14	0.01
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE1	14	0.01
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE2	14	0.01
(1,21)	1:A:12:VAL:HG11	1:B:35:MET:HE3	14	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE1	14	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE2	14	0.01
(1,21)	1:A:12:VAL:HG12	1:B:35:MET:HE3	14	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE1	14	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE2	14	0.01
(1,21)	1:A:12:VAL:HG13	1:B:35:MET:HE3	14	0.01
(1,207)	1:B:16:ILE:HG21	1:A:43:HIS:HD2	1	0.01
(1,207)	1:B:16:ILE:HG22	1:A:43:HIS:HD2	1	0.01
(1,207)	1:B:16:ILE:HG23	1:A:43:HIS:HD2	1	0.01
(1,207)	1:B:16:ILE:HG21	1:A:43:HIS:HD2	4	0.01
(1,207)	1:B:16:ILE:HG22	1:A:43:HIS:HD2	4	0.01
(1,207)	1:B:16:ILE:HG23	1:A:43:HIS:HD2	4	0.01
(1,207)	1:B:16:ILE:HG21	1:A:43:HIS:HD2	10	0.01
(1,207)	1:B:16:ILE:HG22	1:A:43:HIS:HD2	10	0.01
(1,207)	1:B:16:ILE:HG23	1:A:43:HIS:HD2	10	0.01
(1,202)	1:B:16:ILE:HG12	1:A:39:ASN:H	10	0.01
(1,202)	1:B:16:ILE:HG13	1:A:39:ASN:H	10	0.01
(1,202)	1:B:16:ILE:HG12	1:A:39:ASN:H	14	0.01
(1,202)	1:B:16:ILE:HG13	1:A:39:ASN:H	14	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD11	11	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD12	11	0.01
(1,2)	1:A:7:TYR:HB2	1:B:32:LEU:HD13	11	0.01
(1,191)	1:B:15:LEU:HD21	1:A:36:ALA:H	3	0.01
(1,191)	1:B:15:LEU:HD22	1:A:36:ALA:H	3	0.01
(1,191)	1:B:15:LEU:HD23	1:A:36:ALA:H	3	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	3	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	3	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	8	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	8	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	12	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	12	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	14	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	14	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	16	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	16	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	17	0.01
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	17	0.01
(1,19)	1:A:11:GLN:HG2	1:B:32:LEU:HG	19	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,19)	1:A:11:GLN:HG3	1:B:32:LEU:HG	19	0.01
(1,187)	1:B:15:LEU:HD21	1:A:26:HIS:HD2	12	0.01
(1,187)	1:B:15:LEU:HD22	1:A:26:HIS:HD2	12	0.01
(1,187)	1:B:15:LEU:HD23	1:A:26:HIS:HD2	12	0.01
(1,183)	1:B:15:LEU:HD11	1:A:26:HIS:HD2	3	0.01
(1,183)	1:B:15:LEU:HD12	1:A:26:HIS:HD2	3	0.01
(1,183)	1:B:15:LEU:HD13	1:A:26:HIS:HD2	3	0.01
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE1	2	0.01
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE2	2	0.01
(1,175)	1:B:12:VAL:HG11	1:A:35:MET:HE3	2	0.01
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE1	2	0.01
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE2	2	0.01
(1,175)	1:B:12:VAL:HG12	1:A:35:MET:HE3	2	0.01
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE1	2	0.01
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE2	2	0.01
(1,175)	1:B:12:VAL:HG13	1:A:35:MET:HE3	2	0.01
(1,173)	1:B:11:GLN:HG2	1:A:32:LEU:HG	11	0.01
(1,173)	1:B:11:GLN:HG3	1:A:32:LEU:HG	11	0.01
(1,173)	1:B:11:GLN:HG2	1:A:32:LEU:HG	12	0.01
(1,173)	1:B:11:GLN:HG3	1:A:32:LEU:HG	12	0.01
(1,173)	1:B:11:GLN:HG2	1:A:32:LEU:HG	19	0.01
(1,173)	1:B:11:GLN:HG3	1:A:32:LEU:HG	19	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD21	1	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD22	1	0.01
(1,16)	1:A:11:GLN:HE21	1:B:32:LEU:HD23	1	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD21	1	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD22	1	0.01
(1,16)	1:A:11:GLN:HE22	1:B:32:LEU:HD23	1	0.01
(1,1483)	1:B:69:VAL:H	1:B:65:LEU:O	2	0.01
(1,1483)	1:B:69:VAL:H	1:B:65:LEU:O	7	0.01
(1,1483)	1:B:69:VAL:H	1:B:65:LEU:O	16	0.01
(1,1475)	1:B:65:LEU:H	1:B:61:PHE:O	17	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD21	13	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD22	13	0.01
(1,147)	1:A:58:ALA:HB1	1:B:65:LEU:HD23	13	0.01
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD21	13	0.01
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD22	13	0.01
(1,147)	1:A:58:ALA:HB2	1:B:65:LEU:HD23	13	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD21	13	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD22	13	0.01
(1,147)	1:A:58:ALA:HB3	1:B:65:LEU:HD23	13	0.01
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	9	0.01
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	14	0.01
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	18	0.01
(1,1468)	1:B:61:PHE:N	1:B:57:VAL:O	19	0.01
(1,1461)	1:B:58:ALA:H	1:B:54:ARG:O	17	0.01
(1,1457)	1:B:40:CYS:H	1:B:36:ALA:O	13	0.01
(1,1449)	1:B:35:MET:H	1:B:31:ASP:O	17	0.01
(1,1448)	1:B:25:LYS:N	1:B:21:VAL:O	9	0.01
(1,1448)	1:B:25:LYS:N	1:B:21:VAL:O	17	0.01
(1,1443)	1:B:23:LEU:H	1:B:19:ILE:O	1	0.01
(1,1443)	1:B:23:LEU:H	1:B:19:ILE:O	14	0.01
(1,1441)	1:B:22:VAL:H	1:B:18:GLU:O	8	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	5	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	5	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	5	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	5	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	5	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	5	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	8	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	8	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	8	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	8	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	8	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	8	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	10	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	10	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	10	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	10	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	10	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	10	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG21	18	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG22	18	0.01
(1,144)	1:A:55:GLN:HG2	1:B:69:VAL:HG23	18	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG21	18	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG22	18	0.01
(1,144)	1:A:55:GLN:HG3	1:B:69:VAL:HG23	18	0.01
(1,1435)	1:B:19:ILE:H	1:B:15:LEU:O	1	0.01
(1,1435)	1:B:19:ILE:H	1:B:15:LEU:O	18	0.01
(1,1421)	1:A:69:VAL:H	1:A:65:LEU:O	4	0.01
(1,1421)	1:A:69:VAL:H	1:A:65:LEU:O	12	0.01
(1,1421)	1:A:69:VAL:H	1:A:65:LEU:O	16	0.01
(1,1415)	1:A:66:ALA:H	1:A:62:ALA:O	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1409)	1:A:63:LYS:H	1:A:59:GLU:O	18	0.01
(1,1406)	1:A:61:PHE:N	1:A:57:VAL:O	10	0.01
(1,1406)	1:A:61:PHE:N	1:A:57:VAL:O	18	0.01
(1,1401)	1:A:59:GLU:H	1:A:55:GLN:O	6	0.01
(1,1389)	1:A:35:MET:H	1:A:31:ASP:O	2	0.01
(1,1389)	1:A:35:MET:H	1:A:31:ASP:O	5	0.01
(1,1389)	1:A:35:MET:H	1:A:31:ASP:O	15	0.01
(1,1388)	1:A:25:LYS:N	1:A:21:VAL:O	5	0.01
(1,1388)	1:A:25:LYS:N	1:A:21:VAL:O	6	0.01
(1,1388)	1:A:25:LYS:N	1:A:21:VAL:O	12	0.01
(1,1386)	1:A:24:GLU:N	1:A:20:LEU:O	15	0.01
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	2	0.01
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	6	0.01
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	11	0.01
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	17	0.01
(1,1383)	1:A:23:LEU:H	1:A:19:ILE:O	19	0.01
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	3	0.01
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	7	0.01
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	15	0.01
(1,1381)	1:A:22:VAL:H	1:A:18:GLU:O	16	0.01
(1,1375)	1:A:19:ILE:H	1:A:15:LEU:O	7	0.01
(1,1375)	1:A:19:ILE:H	1:A:15:LEU:O	16	0.01
(1,1373)	1:A:18:GLU:H	1:A:14:SER:O	7	0.01
(1,1367)	1:A:15:LEU:H	1:A:11:GLN:O	7	0.01
(1,1364)	1:A:13:GLU:N	1:A:9:ASN:O	8	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD11	8	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD12	8	0.01
(1,1359)	1:B:70:LYS:HA	1:B:73:LEU:HD13	8	0.01
(1,1349)	1:B:68:SER:HA	1:B:70:LYS:H	13	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG21	14	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG22	14	0.01
(1,1336)	1:B:65:LEU:HD11	1:B:69:VAL:HG23	14	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG21	14	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG22	14	0.01
(1,1336)	1:B:65:LEU:HD12	1:B:69:VAL:HG23	14	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG21	14	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG22	14	0.01
(1,1336)	1:B:65:LEU:HD13	1:B:69:VAL:HG23	14	0.01
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	10	0.01
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	10	0.01
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	15	0.01
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	17	0.01
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	17	0.01
(1,1335)	1:B:65:LEU:HB2	1:B:68:SER:H	18	0.01
(1,1335)	1:B:65:LEU:HB3	1:B:68:SER:H	18	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD21	2	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD22	2	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD23	2	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD21	2	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD22	2	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD23	2	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD21	2	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD22	2	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD23	2	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD21	13	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD22	13	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD23	13	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD21	13	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD22	13	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD23	13	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD21	13	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD22	13	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD23	13	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD21	17	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD22	17	0.01
(1,1321)	1:B:62:ALA:HB1	1:B:65:LEU:HD23	17	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD21	17	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD22	17	0.01
(1,1321)	1:B:62:ALA:HB2	1:B:65:LEU:HD23	17	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD21	17	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD22	17	0.01
(1,1321)	1:B:62:ALA:HB3	1:B:65:LEU:HD23	17	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB1	3	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB2	3	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB3	3	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB1	3	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB2	3	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB3	3	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB1	13	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB2	13	0.01
(1,1309)	1:B:61:PHE:HE1	1:B:64:ALA:HB3	13	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB1	13	0.01
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB2	13	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1309)	1:B:61:PHE:HE2	1:B:64:ALA:HB3	13	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB2	2	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB3	2	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB2	2	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB3	2	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB2	13	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB3	13	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB2	13	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB3	13	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB2	17	0.01
(1,1307)	1:B:61:PHE:HD1	1:B:65:LEU:HB3	17	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB2	17	0.01
(1,1307)	1:B:61:PHE:HD2	1:B:65:LEU:HB3	17	0.01
(1,1301)	1:B:60:GLN:HB2	1:B:63:LYS:H	4	0.01
(1,1301)	1:B:60:GLN:HB3	1:B:63:LYS:H	4	0.01
(1,1301)	1:B:60:GLN:HB2	1:B:63:LYS:H	11	0.01
(1,1301)	1:B:60:GLN:HB3	1:B:63:LYS:H	11	0.01
(1,1300)	1:B:60:GLN:HB2	1:B:62:ALA:H	7	0.01
(1,1300)	1:B:60:GLN:HB3	1:B:62:ALA:H	7	0.01
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD2	3	0.01
(1,1297)	1:B:60:GLN:HA	1:B:63:LYS:HD3	3	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB1	8	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB2	8	0.01
(1,1293)	1:B:59:GLU:HG2	1:B:62:ALA:HB3	8	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB1	8	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB2	8	0.01
(1,1293)	1:B:59:GLU:HG3	1:B:62:ALA:HB3	8	0.01
(1,1276)	1:B:57:VAL:HG11	1:B:61:PHE:H	3	0.01
(1,1276)	1:B:57:VAL:HG12	1:B:61:PHE:H	3	0.01
(1,1276)	1:B:57:VAL:HG13	1:B:61:PHE:H	3	0.01
(1,1276)	1:B:57:VAL:HG11	1:B:61:PHE:H	9	0.01
(1,1276)	1:B:57:VAL:HG12	1:B:61:PHE:H	9	0.01
(1,1276)	1:B:57:VAL:HG13	1:B:61:PHE:H	9	0.01
(1,127)	1:A:42:THR:HG21	1:B:68:SER:H	7	0.01
(1,127)	1:A:42:THR:HG22	1:B:68:SER:H	7	0.01
(1,127)	1:A:42:THR:HG23	1:B:68:SER:H	7	0.01
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB2	14	0.01
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB3	14	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB2	14	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB3	14	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB2	14	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB3	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB2	19	0.01
(1,1266)	1:B:56:ALA:HB1	1:B:60:GLN:HB3	19	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB2	19	0.01
(1,1266)	1:B:56:ALA:HB2	1:B:60:GLN:HB3	19	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB2	19	0.01
(1,1266)	1:B:56:ALA:HB3	1:B:60:GLN:HB3	19	0.01
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG2	1	0.01
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG3	1	0.01
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG2	1	0.01
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG3	1	0.01
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG2	1	0.01
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG3	1	0.01
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG2	5	0.01
(1,1265)	1:B:56:ALA:HB1	1:B:59:GLU:HG3	5	0.01
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG2	5	0.01
(1,1265)	1:B:56:ALA:HB2	1:B:59:GLU:HG3	5	0.01
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG2	5	0.01
(1,1265)	1:B:56:ALA:HB3	1:B:59:GLU:HG3	5	0.01
(1,1264)	1:B:56:ALA:HB1	1:B:59:GLU:HB2	13	0.01
(1,1264)	1:B:56:ALA:HB1	1:B:59:GLU:HB3	13	0.01
(1,1264)	1:B:56:ALA:HB2	1:B:59:GLU:HB2	13	0.01
(1,1264)	1:B:56:ALA:HB2	1:B:59:GLU:HB3	13	0.01
(1,1264)	1:B:56:ALA:HB3	1:B:59:GLU:HB2	13	0.01
(1,1264)	1:B:56:ALA:HB3	1:B:59:GLU:HB3	13	0.01
(1,126)	1:A:42:THR:HG21	1:B:65:LEU:HG	13	0.01
(1,126)	1:A:42:THR:HG22	1:B:65:LEU:HG	13	0.01
(1,126)	1:A:42:THR:HG23	1:B:65:LEU:HG	13	0.01
(1,126)	1:A:42:THR:HG21	1:B:65:LEU:HG	17	0.01
(1,126)	1:A:42:THR:HG22	1:B:65:LEU:HG	17	0.01
(1,126)	1:A:42:THR:HG23	1:B:65:LEU:HG	17	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	1	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	1	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	1	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	1	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	1	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	1	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	4	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	4	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	4	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	4	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	4	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	4	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	6	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	6	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	6	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	6	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	6	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	6	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	7	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	7	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	7	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	7	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	7	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	7	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	9	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	9	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	9	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	9	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	9	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	9	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	10	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	10	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	10	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	10	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	10	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	10	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	12	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	12	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	12	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	12	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	12	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	12	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	15	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	15	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	15	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	15	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	15	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	15	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	18	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	18	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	18	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	18	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	18	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	18	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB2	19	0.01
(1,124)	1:A:42:THR:HG21	1:B:65:LEU:HB3	19	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB2	19	0.01
(1,124)	1:A:42:THR:HG22	1:B:65:LEU:HB3	19	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB2	19	0.01
(1,124)	1:A:42:THR:HG23	1:B:65:LEU:HB3	19	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	4	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	4	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	8	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	8	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	9	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	9	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	15	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	15	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	16	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	16	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD2	18	0.01
(1,1229)	1:B:51:SER:H	1:B:54:ARG:HD3	18	0.01
(1,1225)	1:B:51:SER:HB2	1:B:54:ARG:HE	1	0.01
(1,1225)	1:B:51:SER:HB3	1:B:54:ARG:HE	1	0.01
(1,1225)	1:B:51:SER:HB2	1:B:54:ARG:HE	16	0.01
(1,1225)	1:B:51:SER:HB3	1:B:54:ARG:HE	16	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD11	2	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD12	2	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD13	2	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD11	13	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD12	13	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD13	13	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD11	17	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD12	17	0.01
(1,122)	1:A:42:THR:HB	1:B:65:LEU:HD13	17	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD11	5	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD12	5	0.01
(1,120)	1:A:42:THR:HA	1:B:65:LEU:HD13	5	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	1	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	3	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	5	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	8	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	16	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	19	0.01
(1,1189)	1:B:47:ARG:H	1:B:48:LYS:HA	20	0.01
(1,1188)	1:B:47:ARG:HA	1:B:49:VAL:H	5	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG2	14	0.01
(1,1186)	1:B:46:GLU:HG2	1:B:54:ARG:HG3	14	0.01
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG2	14	0.01
(1,1186)	1:B:46:GLU:HG3	1:B:54:ARG:HG3	14	0.01
(1,1185)	1:B:46:GLU:HG2	1:B:54:ARG:HE	17	0.01
(1,1185)	1:B:46:GLU:HG3	1:B:54:ARG:HE	17	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	6	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	6	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	6	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	7	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	7	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	7	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	9	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	9	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	9	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	10	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	10	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	10	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	14	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	14	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	14	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	16	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	16	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	16	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	17	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	17	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	17	0.01
(1,1174)	1:B:45:LEU:HD21	1:B:54:ARG:H	20	0.01
(1,1174)	1:B:45:LEU:HD22	1:B:54:ARG:H	20	0.01
(1,1174)	1:B:45:LEU:HD23	1:B:54:ARG:H	20	0.01
(1,1172)	1:B:45:LEU:HD21	1:B:54:ARG:HD2	8	0.01
(1,1172)	1:B:45:LEU:HD21	1:B:54:ARG:HD3	8	0.01
(1,1172)	1:B:45:LEU:HD22	1:B:54:ARG:HD2	8	0.01
(1,1172)	1:B:45:LEU:HD22	1:B:54:ARG:HD3	8	0.01
(1,1172)	1:B:45:LEU:HD23	1:B:54:ARG:HD2	8	0.01
(1,1172)	1:B:45:LEU:HD23	1:B:54:ARG:HD3	8	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG11	9	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG12	9	0.01
(1,1164)	1:B:45:LEU:HD11	1:B:57:VAL:HG13	9	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG11	9	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG12	9	0.01
(1,1164)	1:B:45:LEU:HD12	1:B:57:VAL:HG13	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG11	9	0.01
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG12	9	0.01
(1,1164)	1:B:45:LEU:HD13	1:B:57:VAL:HG13	9	0.01
(1,1153)	1:B:43:HIS:HD2	1:B:44:LEU:HG	13	0.01
(1,1153)	1:B:43:HIS:HD2	1:B:44:LEU:HG	16	0.01
(1,1152)	1:B:43:HIS:HD2	1:B:44:LEU:HA	13	0.01
(1,1150)	1:B:43:HIS:HA	1:B:47:ARG:H	5	0.01
(1,1150)	1:B:43:HIS:HA	1:B:47:ARG:H	7	0.01
(1,1148)	1:B:42:THR:HG21	1:B:46:GLU:H	13	0.01
(1,1148)	1:B:42:THR:HG22	1:B:46:GLU:H	13	0.01
(1,1148)	1:B:42:THR:HG23	1:B:46:GLU:H	13	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	1	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	1	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	1	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	1	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	1	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	1	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	1	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	1	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	1	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	2	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	2	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	2	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	2	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	2	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	2	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	2	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	2	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	2	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	3	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	3	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	3	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	3	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	3	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	3	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	3	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	3	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	3	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	13	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	13	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	13	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	13	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	13	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	13	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	13	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	13	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	13	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD21	18	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD22	18	0.01
(1,1138)	1:B:41:VAL:HG11	1:B:65:LEU:HD23	18	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD21	18	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD22	18	0.01
(1,1138)	1:B:41:VAL:HG12	1:B:65:LEU:HD23	18	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD21	18	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD22	18	0.01
(1,1138)	1:B:41:VAL:HG13	1:B:65:LEU:HD23	18	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	1	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	1	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	1	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	1	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	1	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	1	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	1	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	1	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	1	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	3	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	3	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	3	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	3	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	3	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	3	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	3	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	3	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	3	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	4	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	4	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	4	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	4	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	4	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	4	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	4	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	4	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	4	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	6	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	6	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	6	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	6	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	6	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	6	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	6	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	6	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	6	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	11	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	11	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	11	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	11	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	11	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	11	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	11	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	11	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	11	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	18	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	18	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	18	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	18	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	18	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	18	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	18	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	18	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	18	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD11	20	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD12	20	0.01
(1,1137)	1:B:41:VAL:HG11	1:B:65:LEU:HD13	20	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD11	20	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD12	20	0.01
(1,1137)	1:B:41:VAL:HG12	1:B:65:LEU:HD13	20	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD11	20	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD12	20	0.01
(1,1137)	1:B:41:VAL:HG13	1:B:65:LEU:HD13	20	0.01
(1,1129)	1:B:41:VAL:HG11	1:B:45:LEU:HB2	20	0.01
(1,1129)	1:B:41:VAL:HG11	1:B:45:LEU:HB3	20	0.01
(1,1129)	1:B:41:VAL:HG12	1:B:45:LEU:HB2	20	0.01
(1,1129)	1:B:41:VAL:HG12	1:B:45:LEU:HB3	20	0.01
(1,1129)	1:B:41:VAL:HG13	1:B:45:LEU:HB2	20	0.01
(1,1129)	1:B:41:VAL:HG13	1:B:45:LEU:HB3	20	0.01
(1,1114)	1:B:40:CYS:HA	1:B:43:HIS:HD2	13	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1114)	1:B:40:CYS:HA	1:B:43:HIS:HD2	16	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	4	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	4	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	7	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	7	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	9	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	9	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	17	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	17	0.01
(1,1107)	1:B:39:ASN:HB2	1:B:42:THR:H	20	0.01
(1,1107)	1:B:39:ASN:HB3	1:B:42:THR:H	20	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB2	4	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB3	4	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB2	4	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB3	4	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB2	4	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB3	4	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB2	17	0.01
(1,1089)	1:B:37:LEU:HD11	1:B:40:CYS:HB3	17	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB2	17	0.01
(1,1089)	1:B:37:LEU:HD12	1:B:40:CYS:HB3	17	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB2	17	0.01
(1,1089)	1:B:37:LEU:HD13	1:B:40:CYS:HB3	17	0.01
(1,1077)	1:B:35:MET:HB2	1:B:39:ASN:HD21	8	0.01
(1,1077)	1:B:35:MET:HB2	1:B:39:ASN:HD22	8	0.01
(1,1077)	1:B:35:MET:HB3	1:B:39:ASN:HD21	8	0.01
(1,1077)	1:B:35:MET:HB3	1:B:39:ASN:HD22	8	0.01
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD21	18	0.01
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD22	18	0.01
(1,1070)	1:B:34:LEU:HD21	1:B:37:LEU:HD23	18	0.01
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD21	18	0.01
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD22	18	0.01
(1,1070)	1:B:34:LEU:HD22	1:B:37:LEU:HD23	18	0.01
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD21	18	0.01
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD22	18	0.01
(1,1070)	1:B:34:LEU:HD23	1:B:37:LEU:HD23	18	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB2	5	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB3	5	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB2	5	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB3	5	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB2	13	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB3	13	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB2	13	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB3	13	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB2	17	0.01
(1,107)	1:A:38:GLY:HA2	1:B:65:LEU:HB3	17	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB2	17	0.01
(1,107)	1:A:38:GLY:HA3	1:B:65:LEU:HB3	17	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE1	11	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE2	11	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE3	11	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE1	11	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE2	11	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE3	11	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE1	16	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE2	16	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE3	16	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE1	16	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE2	16	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE3	16	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE1	19	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE2	19	0.01
(1,1044)	1:B:31:ASP:HB2	1:B:35:MET:HE3	19	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE1	19	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE2	19	0.01
(1,1044)	1:B:31:ASP:HB3	1:B:35:MET:HE3	19	0.01
(1,1003)	1:B:26:HIS:HB3	1:B:28:ALA:H	6	0.01

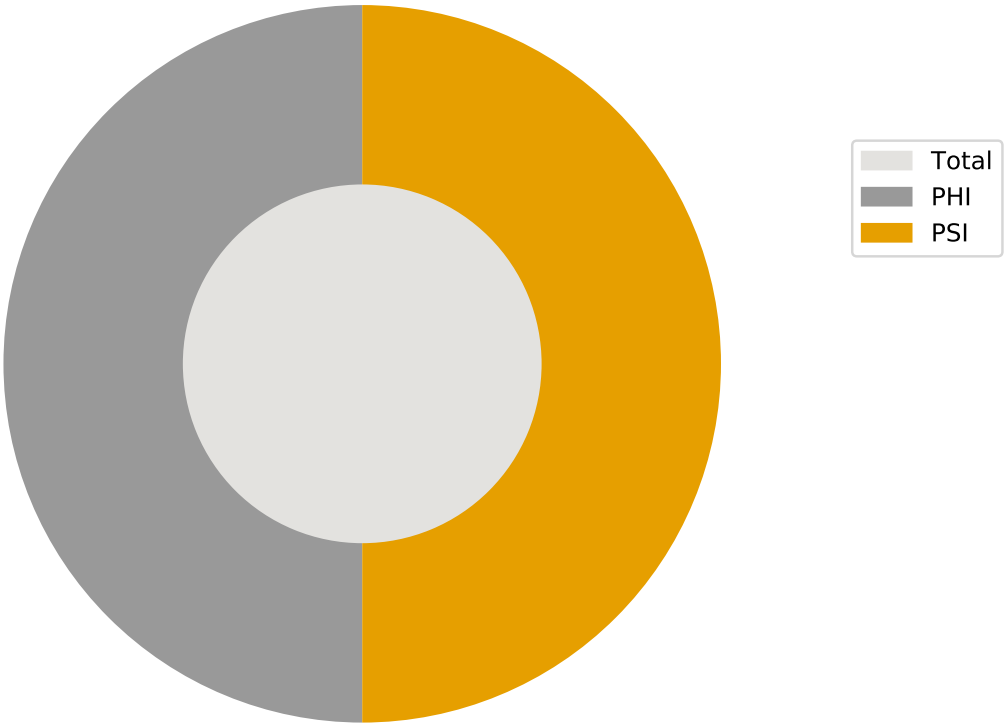
9 Dihedral angle restraints analysis

9.1 Dihedral angle restraints summary

Angle name	Count	%
PHI	126	50.0
PSI	126	50.0
Total	252	100.0

9.1.1 Pie chart : Dihedral angle restraints

There are 0 unmapped restraints



9.2 Dihedral angle violations

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

Angle name	Count	%[1]	%[2]
PHI	10	7.9	52.6
PSI	9	7.1	47.4

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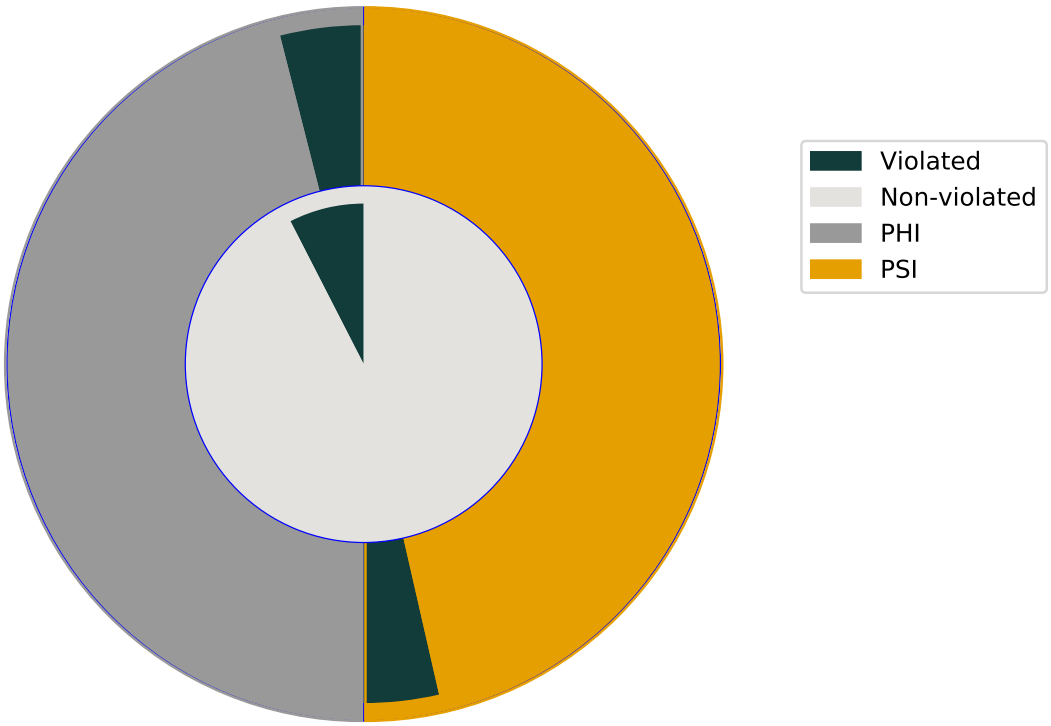
Angle name	Count	%[1]	%[2]
Total	19	7.5	100.0

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

9.2.1 Pie chart : Dihedral angle violations



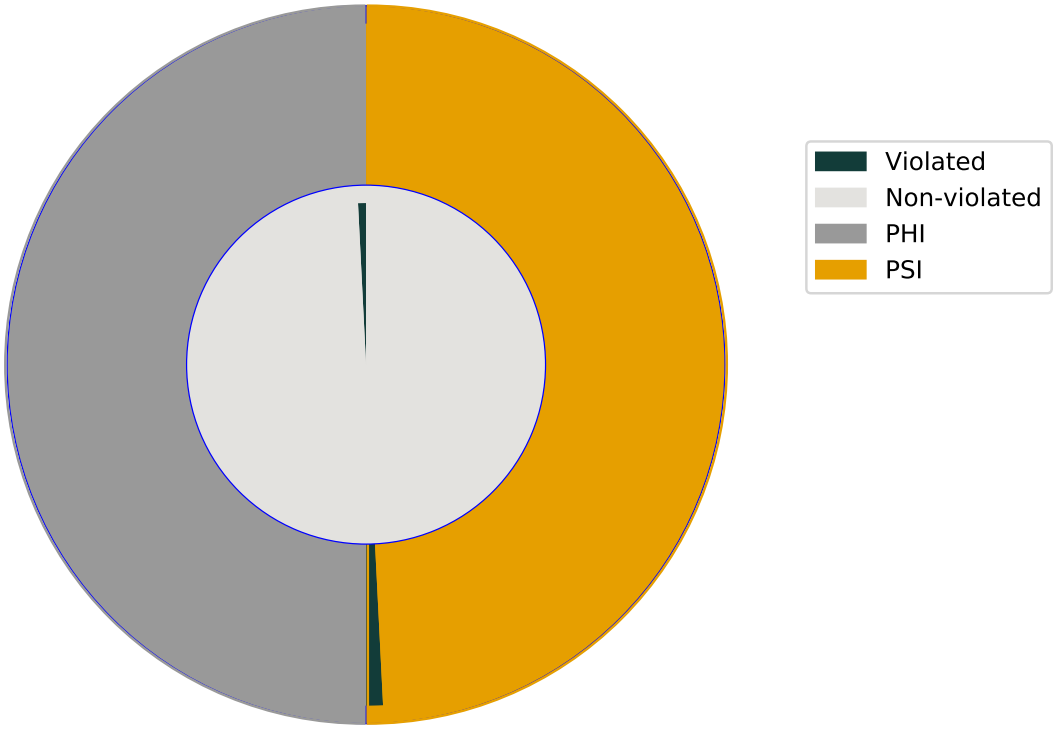
9.3 Consistent dihedral angle violations

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

Angle name	Count	%[1]	%[2]
PHI	0	0.0	0.0
PSI	2	1.6	100.0
Total	2	0.8	100.0

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

9.3.1 Pie chart : Consistent dihedral angle violations



9.4 Residual dihedral angle violations

Violation are counted in different bin sizes and listed below

Range (∘)	Avg. No. of violated restraints per model	Max violation (∘)
0.0-5.0	1.5	1.05
5.0-10.0	None	None
10.0-20.0	None	None
20.0-40.0	2.0	40.0
40.0-80.0	None	None
80.0<	None	None

9.5 Dihedral angle violations in the ensemble

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

No. of violated restraints			No. of violated models
PHI	PSI	Total	
4	4	8	1

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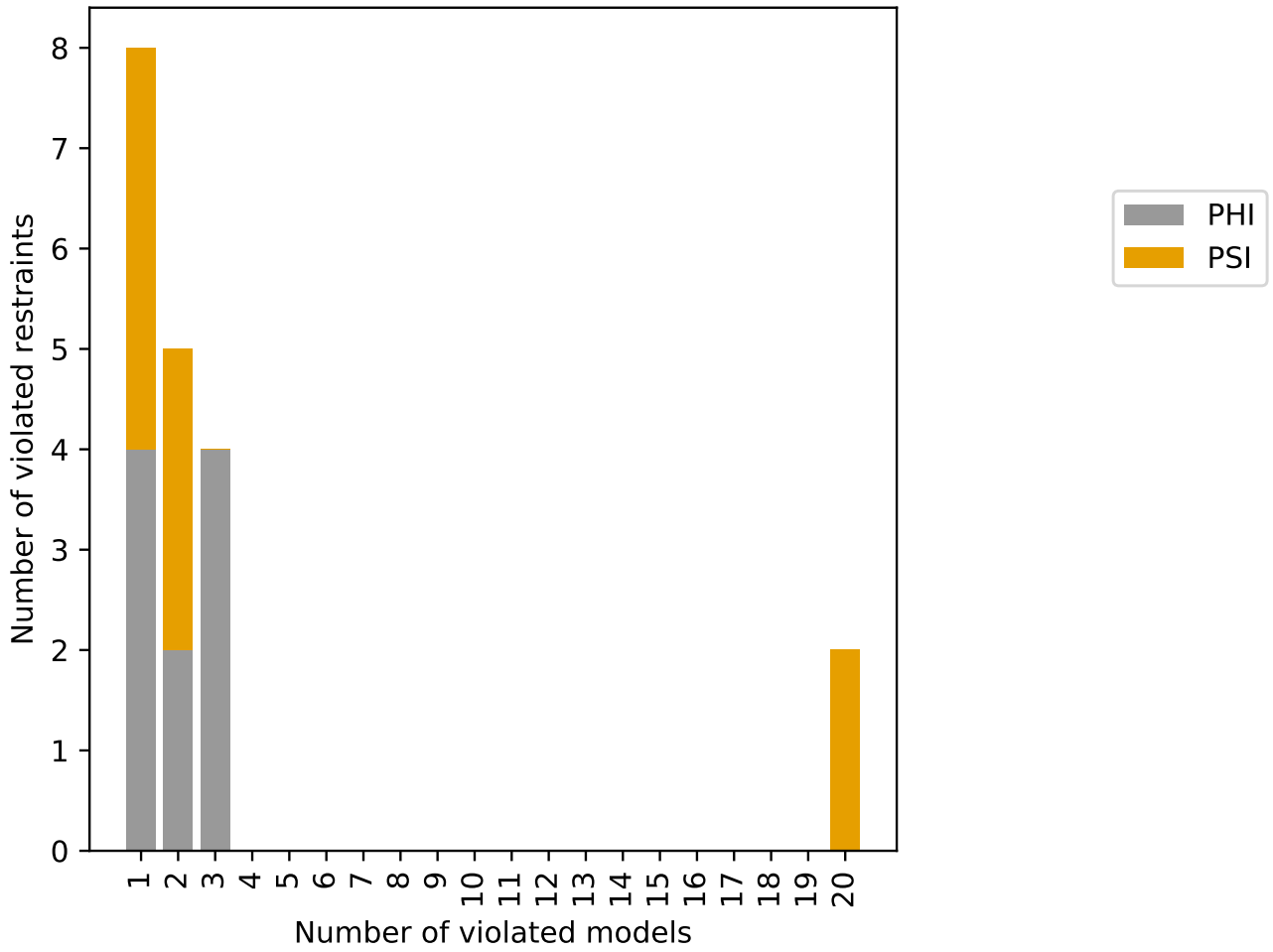
No. of violated restraints			No. of violated models
PHI	PSI	Total	
2	3	5	2
4	0	4	3
0	0	0	4
0	0	0	5
0	0	0	6
0	0	0	7
0	0	0	8
0	0	0	9
0	0	0	10
0	0	0	11
0	0	0	12
0	0	0	13
0	0	0	14
0	0	0	15
0	0	0	16
0	0	0	17
0	0	0	18
0	0	0	19
0	2	2	20

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



9.6 Violations in each model

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

Model ID	No. of violations			Mean (∘)	Max (∘)
	PHI	PSI	Total		
1	2	3	5	12.24	32.64
2	1	2	3	23.54	39.23
3	0	3	3	22.69	36.16
4	2	2	4	19.63	39.31
5	2	3	5	14.52	38.71
6	0	2	2	32.14	33.7
7	0	2	2	34.4	34.43
8	0	2	2	34.63	36.52
9	2	3	5	14.06	39.69

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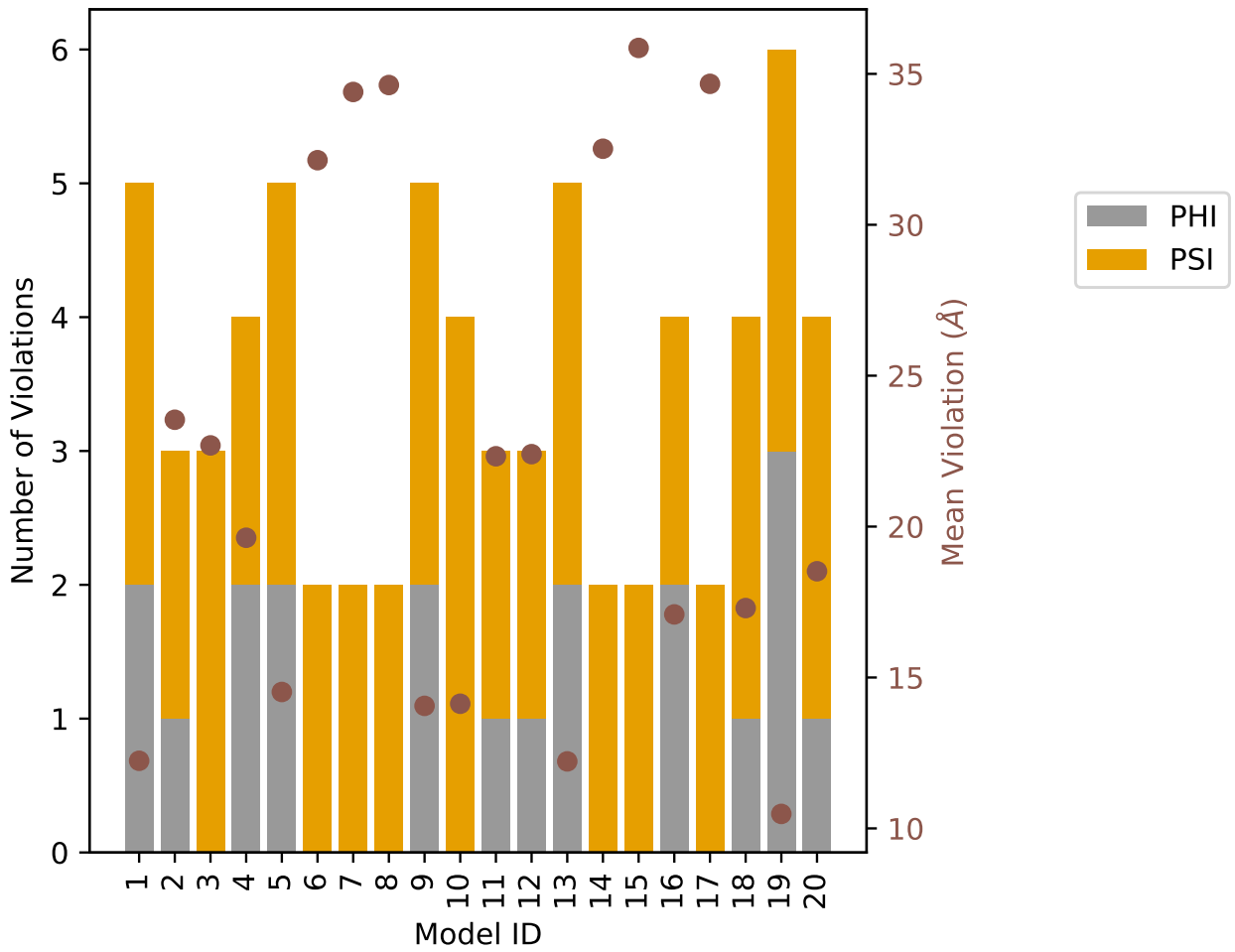
Model ID	No. of violations			Mean (∘)	Max (∘)
	PHI	PSI	Total		
10	0	4	4	14.13	29.02
11	1	2	3	22.33	38.74
12	1	2	3	22.4	33.7
13	2	3	5	12.22	32.05
14	0	2	2	32.52	33.56
15	0	2	2	35.86	39.75
16	2	2	4	17.09	36.6
17	0	2	2	34.67	37.72
18	1	3	4	17.3	38.4
19	3	3	6	10.48	32.98
20	1	3	4	18.52	40.0

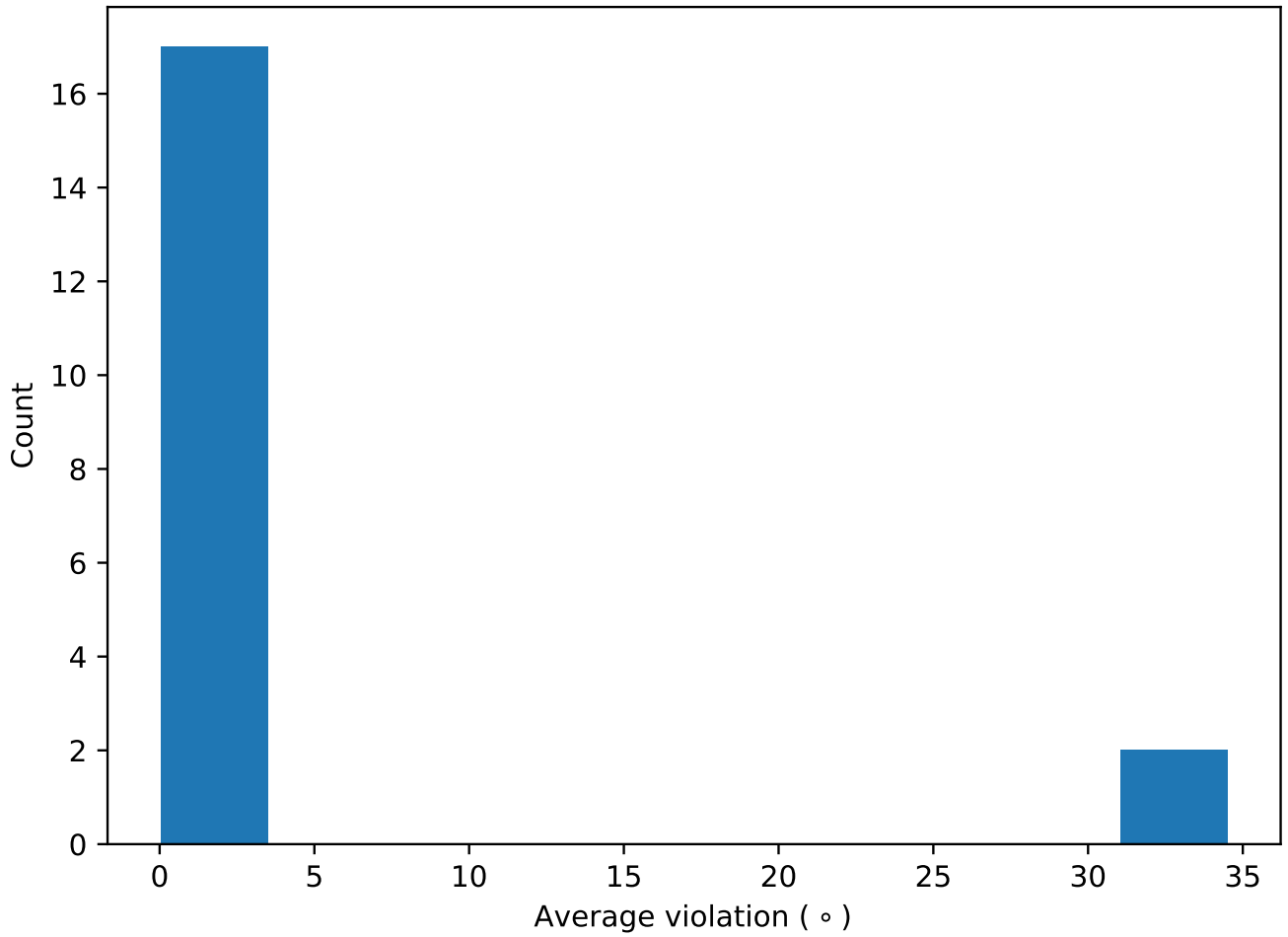
9.6.1 Bar graph : Violations in each model



9.7 Most violated dihedral angle restraints

9.7.1 Histogram : Distribution of mean dihedral angle violations

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



9.7.2 Table: Most violated dihedral angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (∘)	Max (∘)
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	20	34.5	40.0
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	20	33.03	39.31
(1,72)	1:A:46:GLU:N	1:A:46:GLU:CA	1:A:46:GLU:C	1:A:47:ARG:N	1	1.05	1.05
(1,122)	1:A:71:SER:N	1:A:71:SER:CA	1:A:71:SER:C	1:A:72:ASN:N	2	0.27	0.42
(1,200)	1:B:47:ARG:N	1:B:47:ARG:CA	1:B:47:ARG:C	1:B:48:LYS:N	1	0.4	0.4
(1,74)	1:A:47:ARG:N	1:A:47:ARG:CA	1:A:47:ARG:C	1:A:48:LYS:N	2	0.22	0.28
(1,126)	1:A:73:LEU:N	1:A:73:LEU:CA	1:A:73:LEU:C	1:A:74:GLU:N	1	0.09	0.09
(1,124)	1:A:72:ASN:N	1:A:72:ASN:CA	1:A:72:ASN:C	1:A:73:LEU:N	1	0.07	0.07
(1,252)	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	1:B:74:GLU:N	2	0.04	0.05
(1,211)	1:B:52:GLU:C	1:B:53:SER:N	1:B:53:SER:CA	1:B:53:SER:C	3	0.24	0.65

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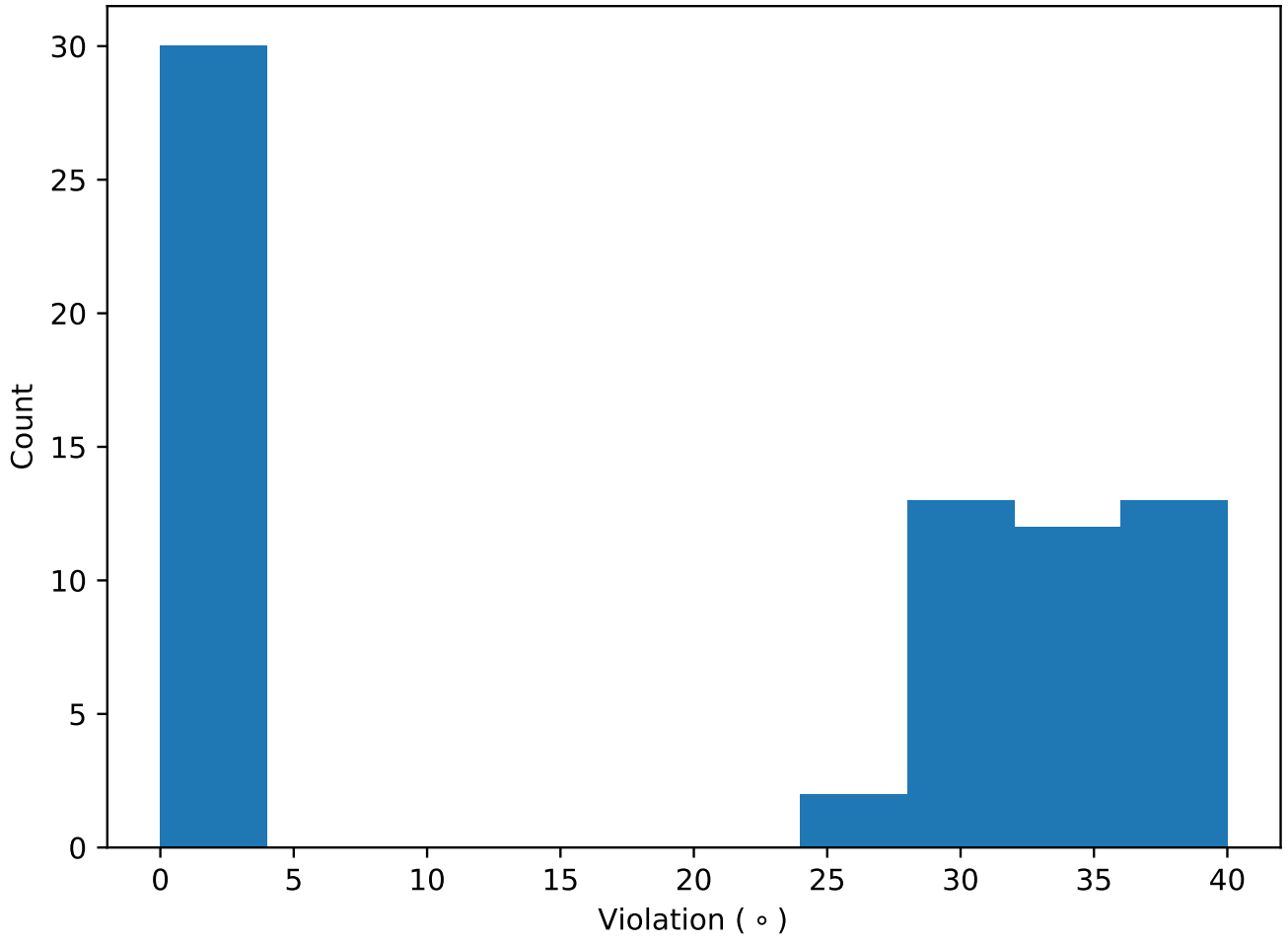
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (◦)	Max (◦)
(1,75)	1:A:47:ARG:C	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	2	0.2	0.37
(1,251)	1:B:72:ASN:C	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	3	0.13	0.34
(1,77)	1:A:48:LYS:C	1:A:49:VAL:N	1:A:49:VAL:CA	1:A:49:VAL:C	3	0.13	0.27
(1,249)	1:B:71:SER:C	1:B:72:ASN:N	1:B:72:ASN:CA	1:B:72:ASN:C	1	0.19	0.19
(1,125)	1:A:72:ASN:C	1:A:73:LEU:N	1:A:73:LEU:CA	1:A:73:LEU:C	2	0.18	0.19
(1,119)	1:A:69:VAL:C	1:A:70:LYS:N	1:A:70:LYS:CA	1:A:70:LYS:C	1	0.09	0.09
(1,203)	1:B:48:LYS:C	1:B:49:VAL:N	1:B:49:VAL:CA	1:B:49:VAL:C	3	0.06	0.09
(1,73)	1:A:46:GLU:C	1:A:47:ARG:N	1:A:47:ARG:CA	1:A:47:ARG:C	1	0.07	0.07
(1,35)	1:A:25:LYS:C	1:A:26:HIS:N	1:A:26:HIS:CA	1:A:26:HIS:C	1	0.06	0.06

9.8 All violated dihedral angleeee restraints

9.8.1 Histogram : Distribution of violations

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



9.8.2 Table: All violated dihedral angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	20	40.0
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	15	39.75
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	9	39.69
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	4	39.31
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	2	39.23
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	11	38.74
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	5	38.71
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	4	38.57
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	18	38.4
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	17	37.72
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	16	36.6
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	8	36.52
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	3	36.16
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	7	34.43
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	7	34.37
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	12	33.7
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	6	33.7
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	14	33.56
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	5	33.49
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	12	33.4
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	19	32.98
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	20	32.96
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	8	32.74
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	1	32.64
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	13	32.05
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	15	31.96
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	3	31.82
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	16	31.67
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	17	31.63
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	14	31.49
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	2	31.21
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	18	30.66
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	6	30.57
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	9	30.16
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	10	29.02
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	19	28.89
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	13	28.87
(1,206)	1:B:50:PRO:N	1:B:50:PRO:CA	1:B:50:PRO:C	1:B:51:SER:N	11	28.17
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	1	27.96
(1,80)	1:A:50:PRO:N	1:A:50:PRO:CA	1:A:50:PRO:C	1:A:51:SER:N	10	27.07
(1,72)	1:A:46:GLU:N	1:A:46:GLU:CA	1:A:46:GLU:C	1:A:47:ARG:N	20	1.05
(1,211)	1:B:52:GLU:C	1:B:53:SER:N	1:B:53:SER:CA	1:B:53:SER:C	19	0.65
(1,122)	1:A:71:SER:N	1:A:71:SER:CA	1:A:71:SER:C	1:A:72:ASN:N	10	0.42
(1,200)	1:B:47:ARG:N	1:B:47:ARG:CA	1:B:47:ARG:C	1:B:48:LYS:N	1	0.4
(1,75)	1:A:47:ARG:C	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	4	0.37
(1,251)	1:B:72:ASN:C	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	9	0.34
(1,74)	1:A:47:ARG:N	1:A:47:ARG:CA	1:A:47:ARG:C	1:A:48:LYS:N	19	0.28
(1,77)	1:A:48:LYS:C	1:A:49:VAL:N	1:A:49:VAL:CA	1:A:49:VAL:C	4	0.27
(1,249)	1:B:71:SER:C	1:B:72:ASN:N	1:B:72:ASN:CA	1:B:72:ASN:C	1	0.19
(1,125)	1:A:72:ASN:C	1:A:73:LEU:N	1:A:73:LEU:CA	1:A:73:LEU:C	2	0.19
(1,125)	1:A:72:ASN:C	1:A:73:LEU:N	1:A:73:LEU:CA	1:A:73:LEU:C	5	0.18
(1,74)	1:A:47:ARG:N	1:A:47:ARG:CA	1:A:47:ARG:C	1:A:48:LYS:N	5	0.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,122)	1:A:71:SER:N	1:A:71:SER:CA	1:A:71:SER:C	1:A:72:ASN:N	18	0.11
(1,77)	1:A:48:LYS:C	1:A:49:VAL:N	1:A:49:VAL:CA	1:A:49:VAL:C	12	0.09
(1,203)	1:B:48:LYS:C	1:B:49:VAL:N	1:B:49:VAL:CA	1:B:49:VAL:C	11	0.09
(1,126)	1:A:73:LEU:N	1:A:73:LEU:CA	1:A:73:LEU:C	1:A:74:GLU:N	3	0.09
(1,119)	1:A:69:VAL:C	1:A:70:LYS:N	1:A:70:LYS:CA	1:A:70:LYS:C	13	0.09
(1,203)	1:B:48:LYS:C	1:B:49:VAL:N	1:B:49:VAL:CA	1:B:49:VAL:C	9	0.08
(1,73)	1:A:46:GLU:C	1:A:47:ARG:N	1:A:47:ARG:CA	1:A:47:ARG:C	16	0.07
(1,124)	1:A:72:ASN:N	1:A:72:ASN:CA	1:A:72:ASN:C	1:A:73:LEU:N	13	0.07
(1,35)	1:A:25:LYS:C	1:A:26:HIS:N	1:A:26:HIS:CA	1:A:26:HIS:C	5	0.06
(1,252)	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	1:B:74:GLU:N	9	0.05
(1,211)	1:B:52:GLU:C	1:B:53:SER:N	1:B:53:SER:CA	1:B:53:SER:C	20	0.05
(1,75)	1:A:47:ARG:C	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	19	0.04
(1,251)	1:B:72:ASN:C	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	18	0.04
(1,77)	1:A:48:LYS:C	1:A:49:VAL:N	1:A:49:VAL:CA	1:A:49:VAL:C	13	0.02
(1,252)	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	1:B:74:GLU:N	10	0.02
(1,251)	1:B:72:ASN:C	1:B:73:LEU:N	1:B:73:LEU:CA	1:B:73:LEU:C	19	0.02
(1,211)	1:B:52:GLU:C	1:B:53:SER:N	1:B:53:SER:CA	1:B:53:SER:C	16	0.02
(1,203)	1:B:48:LYS:C	1:B:49:VAL:N	1:B:49:VAL:CA	1:B:49:VAL:C	1	0.01