wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2KKO
Title	:	Solution NMR structure of the homodimeric winged helix-turn-helix DNA-binding domain (fragment 1-100) Mb0332 from Mycobacterium bovis, a possible ArsR-family transcriptional regulator. Northeast Structural Genomics Consortium Target MbR242E.
Authors	:	Ramelot, T.A.; Cort, J.R.; Wang, D.; Ciccosanti, C.; Jiang, M.; Nair, R.; Rost, B.; Swapna, G.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-06-26

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:

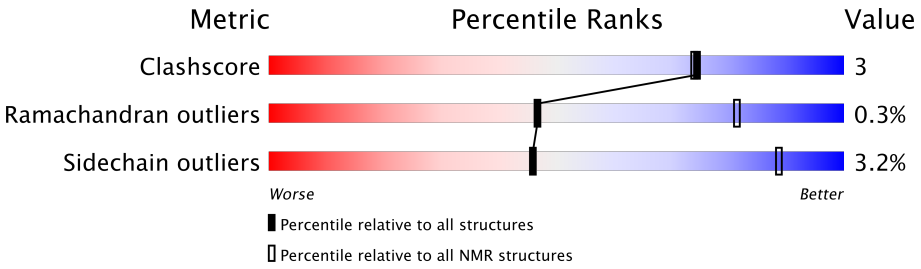
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.6.dev1
BMRB Restraints Analalysis	:	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 63%.

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	108	84% · 14%
1	B	108	83% · 14%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:99, B:8-B:100 (186)	0.55	1

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3328 atoms, of which 1678 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY).

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1664	505	839	165	153	2	
1	B	108	Total	C	H	N	O	S	0
			1664	505	839	165	153	2	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	LEU	-	EXPRESSION TAG	UNP Q7U294
A	102	GLU	-	EXPRESSION TAG	UNP Q7U294
A	103	HIS	-	EXPRESSION TAG	UNP Q7U294
A	104	HIS	-	EXPRESSION TAG	UNP Q7U294
A	105	HIS	-	EXPRESSION TAG	UNP Q7U294
A	106	HIS	-	EXPRESSION TAG	UNP Q7U294
A	107	HIS	-	EXPRESSION TAG	UNP Q7U294
A	108	HIS	-	EXPRESSION TAG	UNP Q7U294
B	101	LEU	-	EXPRESSION TAG	UNP Q7U294
B	102	GLU	-	EXPRESSION TAG	UNP Q7U294
B	103	HIS	-	EXPRESSION TAG	UNP Q7U294
B	104	HIS	-	EXPRESSION TAG	UNP Q7U294
B	105	HIS	-	EXPRESSION TAG	UNP Q7U294
B	106	HIS	-	EXPRESSION TAG	UNP Q7U294
B	107	HIS	-	EXPRESSION TAG	UNP Q7U294
B	108	HIS	-	EXPRESSION TAG	UNP Q7U294

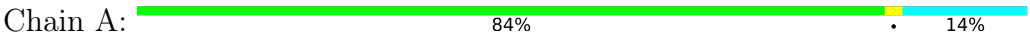
4 Residue-property plots

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.

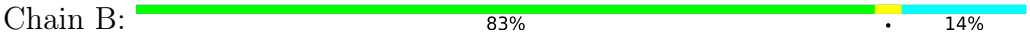
• Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)

Chain A:



• Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)

Chain B:

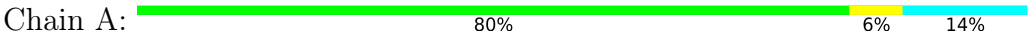


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

• Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)

Chain A:



• Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)

Chain B:


M1
A2
G3
Q4
S5
D6
R7
V15
E38
L59
E69
Y79
R80
E84
R88
L89
E99
H100
L101
E102
H103
H104
H105
H106
H107
H108

5 Refinement protocol and experimental data overview

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

Of the 150 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	2.20
CNS	refinement	1.2

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)	2kko_nmr.cif
Number of chemical shift lists	1
Total number of shifts	2501
Number of shifts mapped to atoms	1563
Number of unparsed shifts	386
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	552
Assignment completeness (well-defined parts)	63%

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	697	730	730	6±3
1	B	696	725	724	6±3
All	All	27860	29100	29080	198

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 3.

5 of 150 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:GLU:HG2	1:B:80:ARG:HB3	0.86	1.48	12	2
1:A:24:ASN:HB2	1:B:16:ALA:HA	0.71	1.60	4	1
1:A:62:LEU:HA	1:A:66:GLY:HA3	0.68	1.62	15	2
1:A:69:GLU:HB2	1:A:82:ALA:HA	0.66	1.65	13	3
1:B:22:LEU:HG	1:B:28:LEU:HD21	0.66	1.68	2	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	93/108 (86%)	91±1 (97±1%)	2±1 (2±1%)	0±0 (0±0%)	47 81
1	B	93/108 (86%)	91±1 (98±1%)	2±1 (2±1%)	0±0 (0±1%)	40 79
All	All	3720/4320 (86%)	3630 (98%)	77 (2%)	13 (0%)	47 81

All 5 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	24	ASN	5
1	B	24	ASN	5
1	B	25	GLY	1
1	B	23	ALA	1
1	A	74	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	67/80 (84%)	65±2 (97±3%)	2±2 (3±3%)	45 88
1	B	67/80 (84%)	65±1 (97±2%)	2±1 (3±2%)	47 89
All	All	2680/3200 (84%)	2594 (97%)	86 (3%)	46 89

5 of 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	38	GLU	6
1	A	24	ASN	6
1	A	38	GLU	5
1	A	69	GLU	5
1	B	69	GLU	4

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 63% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: 2kko_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_2kko.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	2501
Number of shifts mapped to atoms	1563
Number of unparsed shifts	386
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	552
Number of shift outliers (ShiftChecker)	4

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

- Chemical shift has been reported more than once. First 5 (of 386) occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
7	A	2	ALA	HB%	1.410	0.020	1
8	A	2	ALA	HB%	1.410	0.020	1
15	A	3	GLY	HA%	4.030	0.020	1
26	A	4	GLN	HG%	2.390	0.020	1
45	A	6	ASP	HB%	2.710	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 552) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	HIS	HBy	3.42	0.02	2
B	58	ASN	HD2y	6.68	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	LEU	HBx	1.19	0.02	2
A	45	ALA	HB%	1.4	0.02	1
A	84	GLU	HG%	2.35	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
$^{13}C_{\alpha}$	210	-0.46 ± 0.04	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	192	0.10 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	205	-0.28 ± 0.06	None needed (< 0.5 ppm)
^{15}N	206	0.05 ± 0.23	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 63%, i.e. 1406 atoms were assigned a chemical shift out of a possible 2231. 42 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	914/930 (98%)	356/372 (96%)	372/372 (100%)	186/186 (100%)
Sidechain	466/1243 (37%)	68/713 (10%)	374/449 (83%)	24/81 (30%)
Aromatic	26/58 (45%)	13/30 (43%)	13/26 (50%)	0/2 (0%)
Overall	1406/2231 (63%)	437/1115 (39%)	759/847 (90%)	210/269 (78%)

7.1.4 Statistically unusual chemical shifts (i)

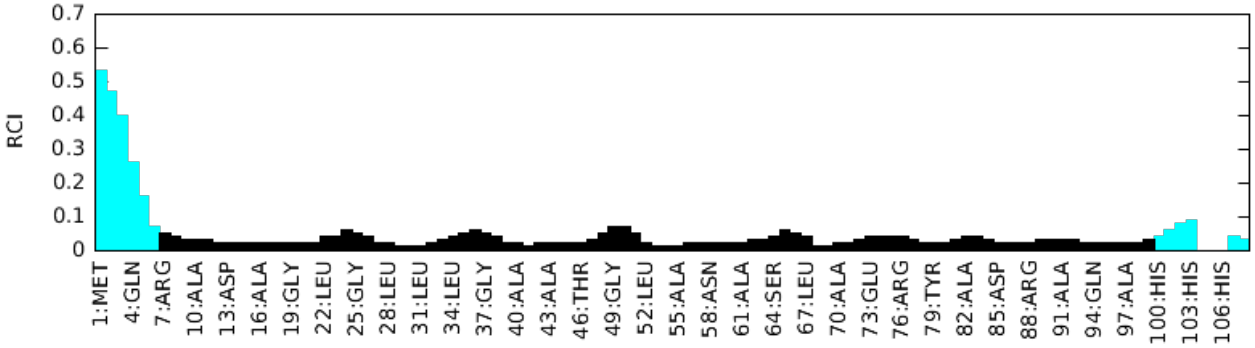
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	1	MET	CB	76.00	44.20 – 21.80	19.2
1	A	1	MET	CB	76.00	44.20 – 21.80	19.2
1	B	1	MET	CA	73.50	67.38 – 44.88	7.7
1	A	1	MET	CA	73.50	67.38 – 44.88	7.7

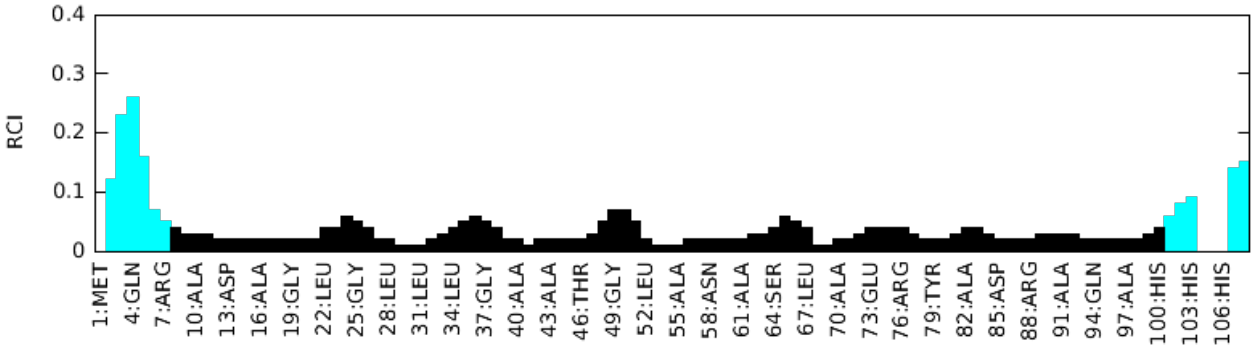
7.1.5 Random Coil Index (RCI) plots

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

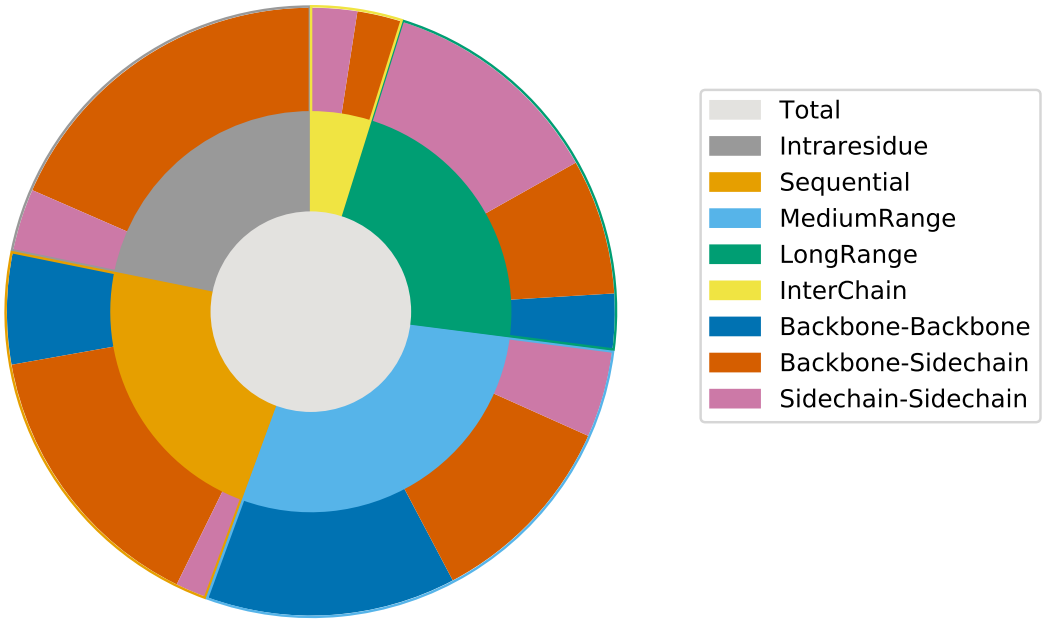
8.1 Distance restraints summary

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)	482(0)	88(0)	570(0)	2.9	21.8
Sequential (|i-j|=1)	156(0)	390(0)	44(0)	590(0)	3.0	22.6
Medium range (|i-j|>1 and |i-j|<5)	348(188)	276(0)	122(0)	746(188)	3.7	28.6
Long range (|i-j|≥5)	78(40)	188(0)	314(0)	580(40)	2.9	22.2
Inter chain	0(0)	62(0)	64(0)	126(0)	0.6	4.8
Total	582(228)	1398(0)	632(0)	2612(228)	13.1	100.0

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

8.1.1 Pie chart : Distance restraints summary



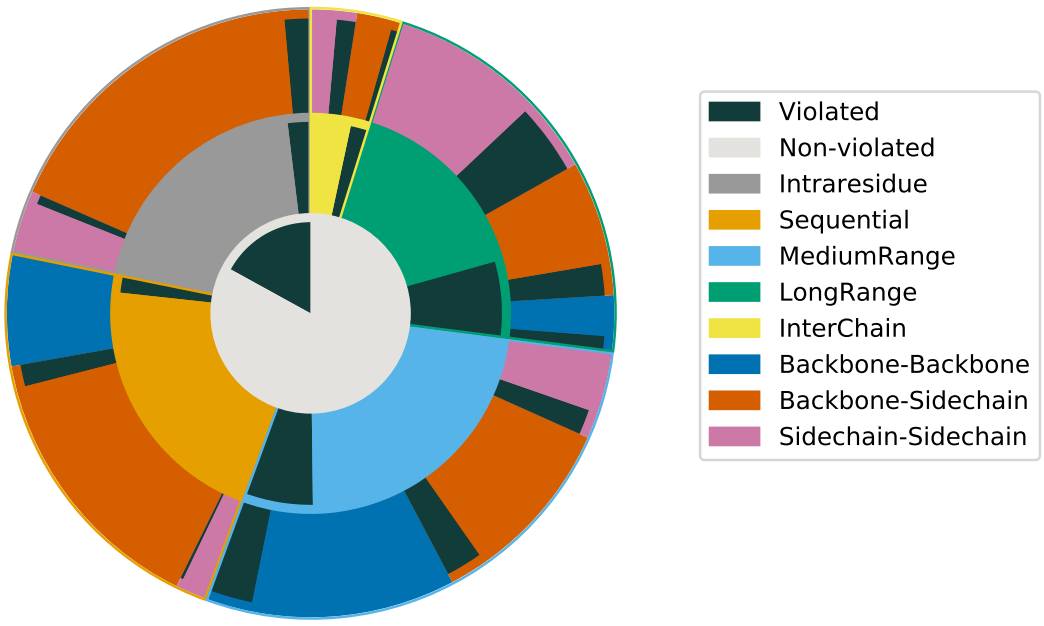
8.2 Distance violations summary

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

Restraints type	B-B[1](%[4])	B-S[2](%[4])	S-S[3](%[4])	Total		
				Total(%[4])	RR[5]	%[6]
Intraresidue (|i-j|=0)	0(0.0)	37(7.7)	13(14.8)	50(8.8)	0.3	11.3
Sequential (|i-j|=1)	3(1.9)	31(7.9)	4(9.1)	38(6.4)	0.2	8.6
Medium range (|i-j|>1 and |i-j|<5)	63(18.1)	52(18.8)	36(29.5)	151(20.2)	0.8	34.0
Long range (|i-j|≥5)	21(26.9)	45(23.9)	101(32.2)	167(28.8)	0.8	37.6
Inter chain	0(0.0)	11(17.7)	27(42.2)	38(30.2)	0.2	8.6
Total	87(14.9)	176(12.6)	181(28.6)	444(17.0)	2.2	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



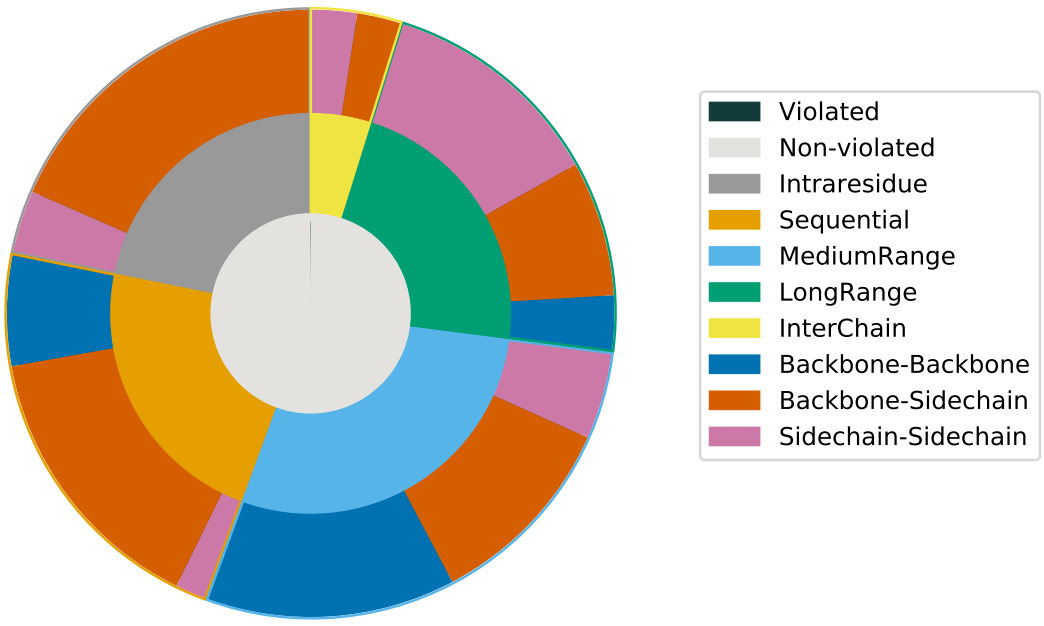
8.3 Consistent distance violations summary

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)	3(0.9)	0(0.0)	0(0.0)	3(0.4)	0.0	100.0
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	3(0.5)	0(0.0)	0(0.0)	3(0.1)	0.0	100.0

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

8.3.1 Pie-chart : Consistent distance violations



8.4 Residual distance violations

Violation are counted in different bin sizes and listed below

Range (Å)	Avg. No. of violated restraints per model	Max violation (Å)
0-0.2	68.0	0.2
0.2-0.5	0.3	0.3
0.5-1.0	None	None
1.0-2.0	None	None
2.0-5.0	None	None
5.0<	None	None

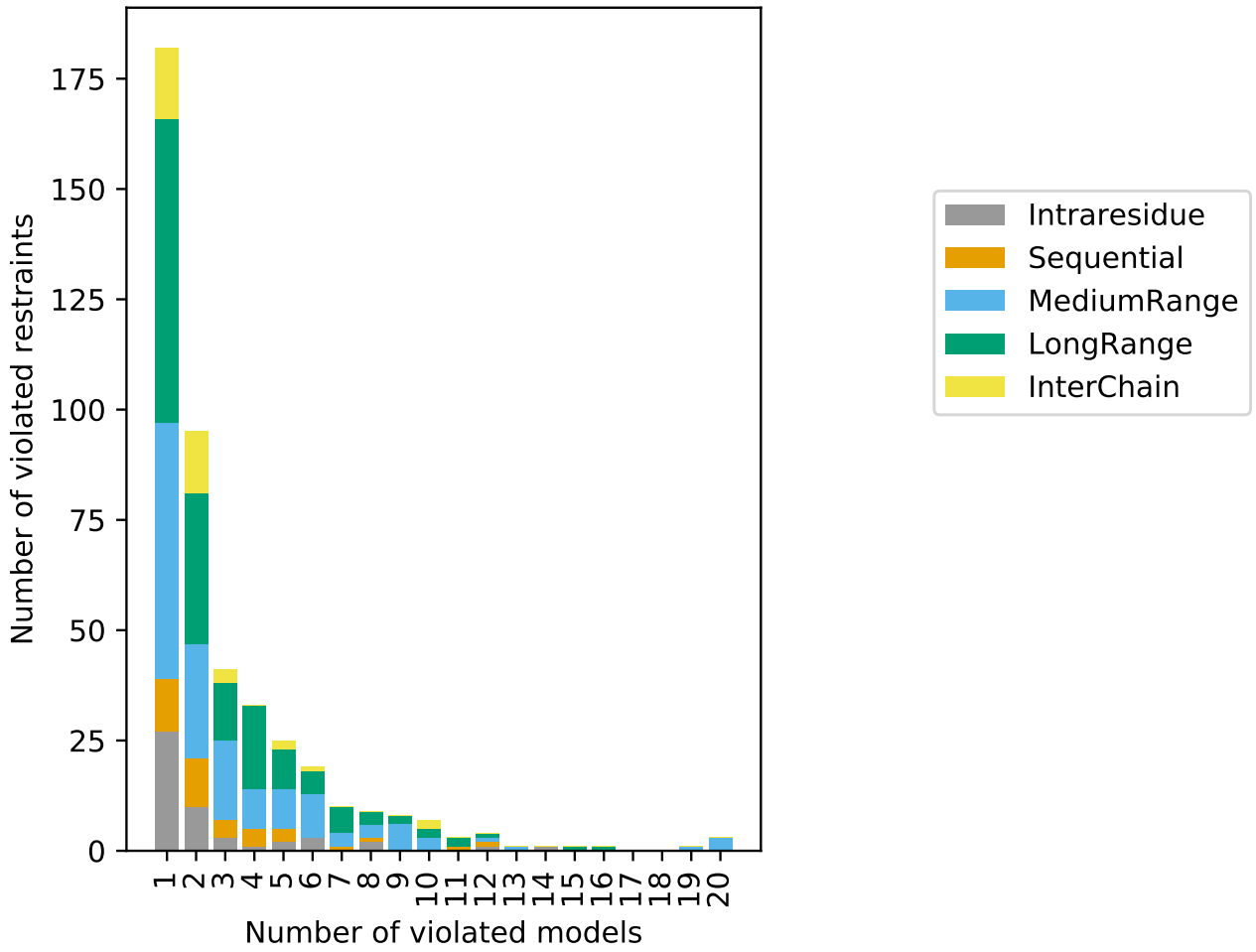
8.5 Distance violations in ensemble

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	
27	12	58	69	16	182	1
10	11	26	34	14	95	2
3	4	18	13	3	41	3
1	4	9	19	0	33	4
2	3	9	9	2	25	5
3	0	10	5	1	19	6
0	1	3	6	0	10	7
2	1	3	3	0	9	8
0	0	6	2	0	8	9
0	0	3	2	2	7	10
0	1	0	2	0	3	11
1	1	1	1	0	4	12
0	0	1	0	0	1	13
1	0	0	0	0	1	14
0	0	0	1	0	1	15
0	0	0	1	0	1	16
0	0	0	0	0	0	17
0	0	0	0	0	0	18
0	0	1	0	0	1	19
0	0	3	0	0	3	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



520 intraresidue restraints, 552 sequential restraints, 595 medium range restraints,413 long range restraints and 88 inter chain restraints are not violated. In total, 2168 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	6	7	22	22	4	61	0.03	0.18
2	9	7	29	25	4	74	0.04	0.16
3	4	8	32	34	1	79	0.04	0.28
4	5	5	27	28	9	74	0.04	0.15
5	6	6	25	25	3	65	0.03	0.17

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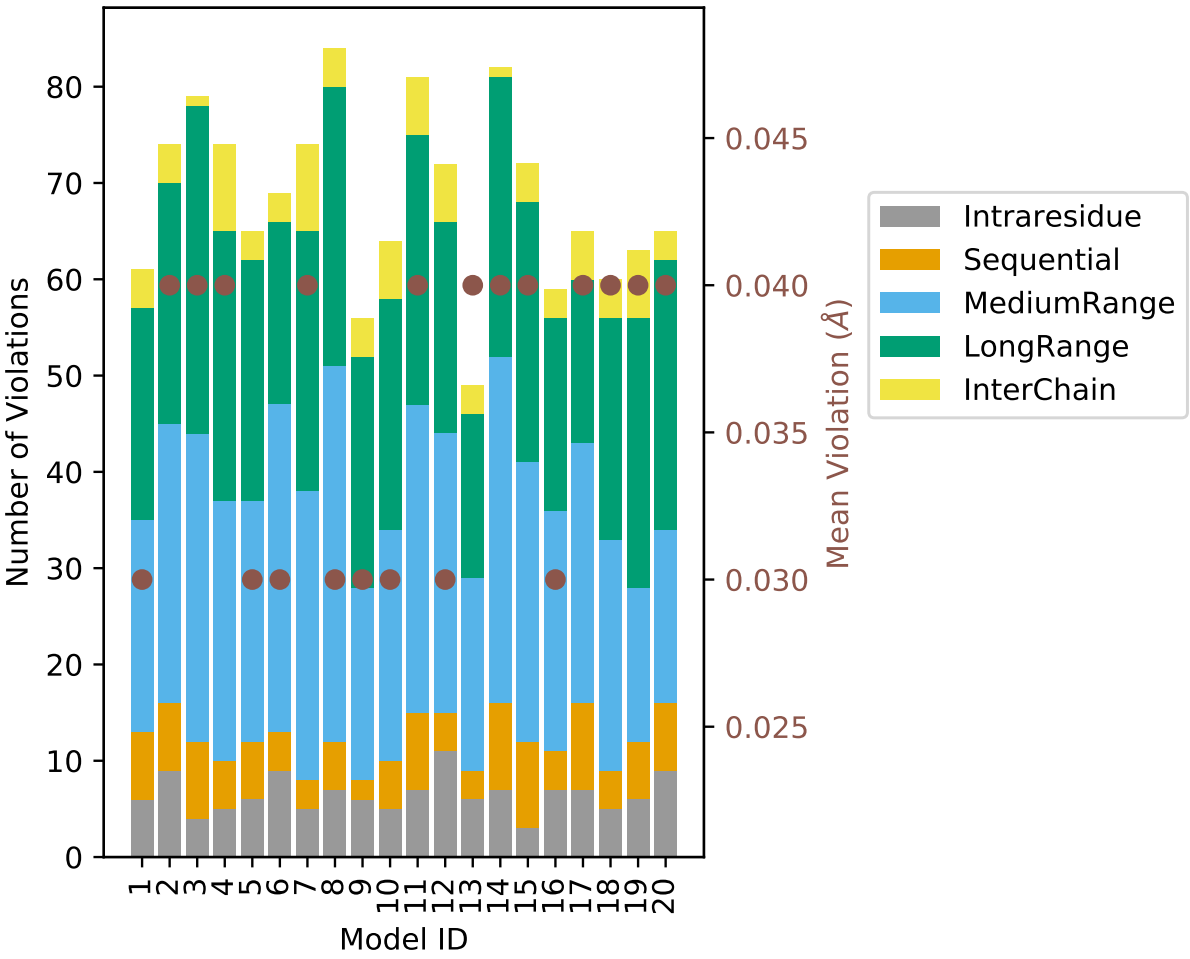
Model ID	No. of violations						Mean (Å)	Max (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total		
6	9	4	34	19	3	69	0.03	0.11
7	5	3	30	27	9	74	0.04	0.11
8	7	5	39	29	4	84	0.03	0.15
9	6	2	20	24	4	56	0.03	0.13
10	5	5	24	24	6	64	0.03	0.13
11	7	8	32	28	6	81	0.04	0.2
12	11	4	29	22	6	72	0.03	0.18
13	6	3	20	17	3	49	0.04	0.18
14	7	9	36	29	1	82	0.04	0.25
15	3	9	29	27	4	72	0.04	0.3
16	7	4	25	20	3	59	0.03	0.18
17	7	9	27	17	5	65	0.04	0.21
18	5	4	24	23	4	60	0.04	0.14
19	6	6	16	28	7	63	0.04	0.13
20	9	7	18	28	3	65	0.04	0.17

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

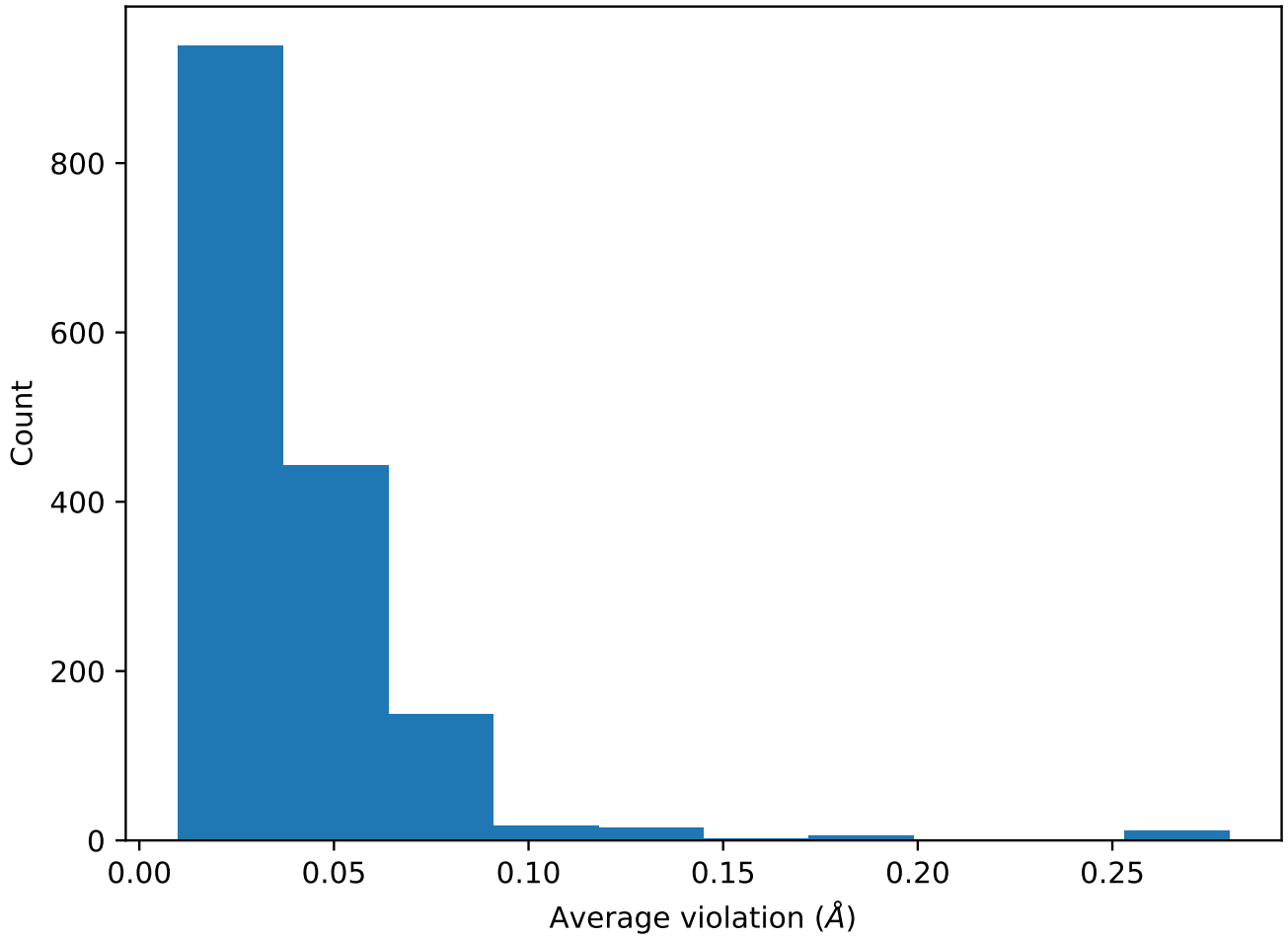
8.6.1 Bar graph : Violations in each model



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)
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	20	0.03	0.05
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	20	0.03	0.06
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	20	0.03	0.05
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	19	0.02	0.04
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	16	0.06	0.13
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	16	0.06	0.13

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	16	0.06	0.13
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	15	0.04	0.1
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	15	0.04	0.1
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	15	0.04	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	15	0.04	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	15	0.04	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	15	0.04	0.1
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	14	0.07	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	14	0.07	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	14	0.07	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	14	0.07	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	14	0.07	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	14	0.07	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	14	0.07	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	14	0.07	0.14
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	13	0.03	0.06
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	12	0.03	0.06
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	12	0.06	0.16
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	12	0.06	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	12	0.08	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	12	0.08	0.16
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	12	0.02	0.06
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	12	0.02	0.06
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	12	0.02	0.06
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	12	0.02	0.06
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	12	0.02	0.06
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	12	0.02	0.06
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	11	0.06	0.11
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	11	0.06	0.11
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	11	0.06	0.11
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	11	0.03	0.07
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	11	0.03	0.07
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	11	0.03	0.07
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	11	0.03	0.07
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	11	0.03	0.07
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	11	0.03	0.07

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	11	0.03	0.07
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	11	0.03	0.07
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	10	0.04	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	10	0.04	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	10	0.04	0.08
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	10	0.03	0.06
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	10	0.03	0.06
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	10	0.03	0.06
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	10	0.03	0.06
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	10	0.03	0.06
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	10	0.03	0.06
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	10	0.02	0.06
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	10	0.03	0.07
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	10	0.02	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	10	0.04	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	10	0.04	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	10	0.04	0.07
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	10	0.02	0.04
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	10	0.02	0.04
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	10	0.02	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	9	0.04	0.1
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	9	0.04	0.1
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	9	0.04	0.1
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	9	0.06	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	9	0.06	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	9	0.06	0.15
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	9	0.03	0.06
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	9	0.02	0.03
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	9	0.03	0.06
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	9	0.03	0.1
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	9	0.02	0.04
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	9	0.06	0.12
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	9	0.06	0.12
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	9	0.06	0.12
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	8	0.03	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	8	0.03	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	8	0.03	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	8	0.03	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	8	0.03	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	8	0.03	0.05
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	8	0.04	0.07
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	8	0.04	0.07
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	8	0.04	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	8	0.04	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	8	0.04	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	8	0.04	0.07
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	8	0.03	0.1
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	8	0.01	0.03
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	8	0.04	0.08
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	8	0.04	0.08
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	8	0.04	0.08
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	8	0.04	0.08
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	8	0.02	0.04
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	8	0.02	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	8	0.02	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	8	0.02	0.04
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	8	0.04	0.07
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	8	0.04	0.07
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	8	0.04	0.07
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	8	0.08	0.15
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	8	0.08	0.15
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	8	0.08	0.15
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	8	0.06	0.15
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	8	0.06	0.15
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	7	0.04	0.07
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	7	0.04	0.07
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	7	0.04	0.07
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	7	0.03	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	7	0.03	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	7	0.03	0.06
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	7	0.03	0.07
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	7	0.02	0.03
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	7	0.03	0.06
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	7	0.02	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	7	0.06	0.13

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	7	0.06	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	7	0.06	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	7	0.06	0.13
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	7	0.04	0.08
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	7	0.04	0.08
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	7	0.04	0.08
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	7	0.04	0.08
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	7	0.05	0.1
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	7	0.05	0.1
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	7	0.05	0.1
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	7	0.05	0.1
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	7	0.03	0.05
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	7	0.03	0.05
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	7	0.03	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	7	0.03	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	7	0.03	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	7	0.03	0.05
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	6	0.03	0.06
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	6	0.03	0.06
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	6	0.03	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	6	0.03	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	6	0.03	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	6	0.03	0.06
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	6	0.02	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	6	0.02	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	6	0.02	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	6	0.02	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	6	0.02	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	6	0.02	0.04
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	6	0.05	0.12
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	6	0.05	0.12
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	6	0.05	0.12
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	6	0.05	0.12
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	6	0.05	0.12
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	6	0.05	0.12
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	6	0.06	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	6	0.06	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	6	0.06	0.09

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	6	0.06	0.09
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	6	0.02	0.06
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	6	0.02	0.03
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	6	0.02	0.04
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	6	0.01	0.02
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	6	0.02	0.04
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	6	0.02	0.03
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	6	0.01	0.03
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	6	0.02	0.03
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	6	0.07	0.12
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	6	0.07	0.12
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	6	0.03	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	6	0.03	0.04
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	6	0.04	0.08
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	6	0.04	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	6	0.04	0.13
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	6	0.02	0.05
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	6	0.02	0.05
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	6	0.02	0.05
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	6	0.11	0.21
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	6	0.11	0.21
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	6	0.03	0.07
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	6	0.03	0.07
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	6	0.03	0.07
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	6	0.03	0.07
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	5	0.03	0.06
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	5	0.03	0.06
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	5	0.03	0.06
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	5	0.03	0.06
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	5	0.05	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	5	0.05	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	5	0.05	0.07
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	5	0.03	0.06
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	5	0.03	0.06
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	5	0.03	0.06
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	5	0.03	0.06
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	5	0.04	0.07
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	5	0.04	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	5	0.06	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	5	0.06	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	5	0.06	0.1

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	5	0.03	0.04
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	5	0.03	0.04
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	5	0.03	0.04
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	5	0.03	0.04
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	5	0.03	0.04
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	5	0.03	0.04
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	5	0.03	0.04
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	5	0.01	0.02
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	5	0.03	0.08
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	5	0.03	0.08
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	5	0.03	0.08
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	5	0.03	0.08
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	5	0.01	0.02
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	5	0.01	0.01
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	5	0.03	0.05
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	5	0.02	0.03
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	5	0.04	0.06
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	5	0.01	0.02
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	5	0.02	0.04
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	5	0.02	0.04
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	5	0.07	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	5	0.07	0.12

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	5	0.04	0.06
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	5	0.04	0.06
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	5	0.04	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	5	0.04	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	5	0.04	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	5	0.04	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	5	0.06	0.08
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	5	0.06	0.08
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	5	0.06	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	5	0.06	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	5	0.06	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	5	0.06	0.08
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	5	0.04	0.06
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	5	0.04	0.06
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	5	0.02	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	5	0.02	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	5	0.05	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	5	0.05	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	5	0.05	0.13
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	5	0.03	0.04
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	5	0.03	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	5	0.03	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	5	0.03	0.04
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	5	0.05	0.13
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	5	0.05	0.13
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	5	0.05	0.13
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	5	0.03	0.05
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	5	0.03	0.05
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	5	0.03	0.05
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	4	0.05	0.08
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG3	4	0.05	0.08
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	4	0.05	0.08

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG3	4	0.05	0.08
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	4	0.06	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	4	0.06	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	4	0.06	0.09
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB1	4	0.02	0.03
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB2	4	0.02	0.03
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB3	4	0.02	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB1	4	0.02	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB2	4	0.02	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB3	4	0.02	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	4	0.02	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	4	0.02	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	4	0.02	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	4	0.02	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	4	0.02	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	4	0.02	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	4	0.02	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	4	0.02	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	4	0.02	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	4	0.02	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	4	0.02	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	4	0.02	0.03
(1,541)	1:A:40:ALA:HA	1:A:78:TYR:HA	4	0.03	0.05
(1,474)	1:A:33:LEU:HG	1:A:39:ARG:HE	4	0.04	0.07
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE1	4	0.04	0.06
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE2	4	0.04	0.06
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE3	4	0.04	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE1	4	0.04	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE2	4	0.04	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE3	4	0.04	0.06
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	4	0.07	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	4	0.07	0.11
(1,2601)	1:B:94:GLN:H	1:B:90:PHE:O	4	0.01	0.02
(1,2583)	1:B:80:ARG:H	1:B:69:GLU:O	4	0.02	0.03
(1,2549)	1:B:57:ALA:H	1:B:53:THR:O	4	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2505)	1:B:16:ALA:H	1:B:12:LEU:O	4	0.01	0.02
(1,2493)	1:A:97:ALA:H	1:A:93:VAL:O	4	0.02	0.03
(1,2469)	1:A:80:ARG:H	1:A:69:GLU:O	4	0.02	0.03
(1,2403)	1:A:22:LEU:H	1:A:18:VAL:O	4	0.03	0.05
(1,2270)	1:B:89:LEU:HD21	1:B:93:VAL:HB	4	0.06	0.12
(1,2270)	1:B:89:LEU:HD22	1:B:93:VAL:HB	4	0.06	0.12
(1,2270)	1:B:89:LEU:HD23	1:B:93:VAL:HB	4	0.06	0.12
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD21	4	0.02	0.04
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD22	4	0.02	0.04
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD23	4	0.02	0.04
(1,2129)	1:B:74:GLY:HA2	1:B:75:THR:HB	4	0.02	0.04
(1,2129)	1:B:74:GLY:HA3	1:B:75:THR:HB	4	0.02	0.04
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	4	0.05	0.09
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE2	4	0.05	0.09
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE1	4	0.05	0.09
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE2	4	0.05	0.09
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG21	4	0.02	0.03
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG22	4	0.02	0.03
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG23	4	0.02	0.03
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	4	0.04	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	4	0.04	0.07
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	4	0.01	0.03
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	4	0.01	0.03
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	4	0.01	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD11	4	0.02	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD12	4	0.02	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD13	4	0.02	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD21	4	0.02	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD22	4	0.02	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD23	4	0.02	0.04
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE1	4	0.03	0.07
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE2	4	0.03	0.07
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	4	0.03	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	4	0.03	0.05
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG21	4	0.04	0.08

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG22	4	0.04	0.08
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG23	4	0.04	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG21	4	0.04	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG22	4	0.04	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG23	4	0.04	0.08
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	4	0.03	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	4	0.03	0.05
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD2	4	0.05	0.07
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD3	4	0.05	0.07
(1,1279)	1:B:8:LYS:HB2	1:B:9:ALA:H	4	0.02	0.03
(1,1279)	1:B:8:LYS:HB3	1:B:9:ALA:H	4	0.02	0.03
(1,1180)	1:A:93:VAL:HG11	1:A:94:GLN:H	4	0.02	0.05
(1,1180)	1:A:93:VAL:HG12	1:A:94:GLN:H	4	0.02	0.05
(1,1180)	1:A:93:VAL:HG13	1:A:94:GLN:H	4	0.02	0.05
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	4	0.02	0.03
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE22	4	0.02	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	4	0.02	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE22	4	0.02	0.03
(1,1000)	1:A:74:GLY:HA2	1:A:75:THR:HB	4	0.01	0.02
(1,1000)	1:A:74:GLY:HA3	1:A:75:THR:HB	4	0.01	0.02
(1,941)	1:A:69:GLU:HG3	1:A:82:ALA:HA	3	0.03	0.03
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	3	0.07	0.1
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	3	0.07	0.1
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	3	0.07	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	3	0.07	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	3	0.07	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	3	0.07	0.1
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG11	3	0.02	0.05
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG12	3	0.02	0.05
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG13	3	0.02	0.05
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	3	0.02	0.03
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	3	0.02	0.03
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	3	0.02	0.03
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	3	0.02	0.03
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	3	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	3	0.02	0.03
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG2	3	0.06	0.1
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG3	3	0.06	0.1
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	3	0.02	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	3	0.02	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	3	0.02	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	3	0.02	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	3	0.02	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	3	0.02	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	3	0.02	0.02
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG2	3	0.02	0.03
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG3	3	0.02	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	3	0.02	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE2	3	0.02	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	3	0.02	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE2	3	0.02	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	3	0.02	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE2	3	0.02	0.03
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	3	0.09	0.2
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA3	3	0.09	0.2
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	3	0.09	0.2
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA3	3	0.09	0.2
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	3	0.09	0.2
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA3	3	0.09	0.2
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	3	0.03	0.05
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	3	0.03	0.05
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	3	0.03	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD21	3	0.03	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD22	3	0.03	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD23	3	0.03	0.05
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	3	0.04	0.08
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB3	3	0.04	0.08
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB2	3	0.04	0.08
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB3	3	0.04	0.08
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	3	0.05	0.08
(1,2591)	1:B:89:LEU:H	1:B:85:ASP:O	3	0.01	0.01
(1,2587)	1:B:87:ALA:H	1:B:83:GLY:O	3	0.02	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2551)	1:B:58:ASN:H	1:B:54:THR:O	3	0.02	0.03
(1,2473)	1:A:87:ALA:H	1:A:83:GLY:O	3	0.01	0.02
(1,2459)	1:A:71:ARG:H	1:A:78:TYR:O	3	0.01	0.02
(1,2421)	1:A:46:THR:H	1:A:42:GLU:O	3	0.01	0.01
(1,2378)	1:B:101:LEU:HD21	1:B:102:GLU:H	3	0.11	0.21
(1,2378)	1:B:101:LEU:HD22	1:B:102:GLU:H	3	0.11	0.21
(1,2378)	1:B:101:LEU:HD23	1:B:102:GLU:H	3	0.11	0.21
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD21	3	0.04	0.05
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD22	3	0.04	0.05
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD23	3	0.04	0.05
(1,2351)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	3	0.04	0.07
(1,2351)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	3	0.04	0.07
(1,2351)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	3	0.04	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG11	3	0.07	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG12	3	0.07	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG13	3	0.07	0.07
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	3	0.03	0.05
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA3	3	0.03	0.05
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	3	0.03	0.04
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE2	3	0.03	0.04
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	3	0.03	0.04
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE2	3	0.03	0.04
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD21	3	0.05	0.08
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD22	3	0.05	0.08
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD23	3	0.05	0.08
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG2	3	0.04	0.08
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG3	3	0.04	0.08
(1,1876)	1:B:53:THR:HG21	1:B:54:THR:H	3	0.05	0.06
(1,1876)	1:B:53:THR:HG22	1:B:54:THR:H	3	0.05	0.06
(1,1876)	1:B:53:THR:HG23	1:B:54:THR:H	3	0.05	0.06
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	3	0.03	0.05
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	3	0.03	0.05
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	3	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	3	0.02	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	3	0.02	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	3	0.03	0.05
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	3	0.03	0.05
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	3	0.03	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB1	3	0.03	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB2	3	0.03	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB3	3	0.03	0.05
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	3	0.02	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	3	0.02	0.02
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE1	3	0.02	0.03
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE2	3	0.02	0.03
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE3	3	0.02	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE1	3	0.02	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE2	3	0.02	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE3	3	0.02	0.03
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG2	3	0.19	0.3
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG3	3	0.19	0.3
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA2	3	0.04	0.06
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA3	3	0.04	0.06
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	3	0.07	0.09
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	3	0.07	0.09
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	3	0.07	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	3	0.07	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	3	0.07	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	3	0.07	0.09
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	3	0.04	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	3	0.04	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	3	0.04	0.05
(1,1217)	1:A:96:VAL:HA	1:A:100:HIS:HD2	3	0.07	0.11
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	3	0.09	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	3	0.09	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	3	0.09	0.14
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	3	0.04	0.05
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	3	0.04	0.05
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	3	0.04	0.05
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	3	0.04	0.05
(1,1062)	1:A:81:ILE:HG21	1:A:83:GLY:H	3	0.01	0.02
(1,1062)	1:A:81:ILE:HG22	1:A:83:GLY:H	3	0.01	0.02
(1,1062)	1:A:81:ILE:HG23	1:A:83:GLY:H	3	0.01	0.02
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	3	0.02	0.03
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	3	0.02	0.03
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	3	0.02	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	2	0.02	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	2	0.02	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	2	0.02	0.03
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB3	2	0.02	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB3	2	0.02	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB1	2	0.02	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB2	2	0.02	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB3	2	0.02	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	2	0.03	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	2	0.03	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	2	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	2	0.04	0.06
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	2	0.04	0.06
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	2	0.04	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD11	2	0.04	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD12	2	0.04	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD13	2	0.04	0.06
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD11	2	0.08	0.12
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD12	2	0.08	0.12
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD13	2	0.08	0.12
(1,863)	1:A:63:LYS:HE2	1:A:70:ALA:H	2	0.04	0.05
(1,863)	1:A:63:LYS:HE3	1:A:70:ALA:H	2	0.04	0.05
(1,861)	1:A:63:LYS:HE2	1:A:69:GLU:HA	2	0.04	0.05
(1,861)	1:A:63:LYS:HE3	1:A:69:GLU:HA	2	0.04	0.05
(1,843)	1:A:62:LEU:HD11	1:A:63:LYS:H	2	0.01	0.01
(1,843)	1:A:62:LEU:HD12	1:A:63:LYS:H	2	0.01	0.01
(1,843)	1:A:62:LEU:HD13	1:A:63:LYS:H	2	0.01	0.01
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	2	0.26	0.26
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	2	0.26	0.26
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	2	0.26	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD21	2	0.26	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD22	2	0.26	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD23	2	0.26	0.26
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD21	2	0.08	0.09
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD22	2	0.08	0.09
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD23	2	0.08	0.09
(1,822)	1:A:60:GLN:HG2	1:A:61:ALA:HA	2	0.04	0.04
(1,822)	1:A:60:GLN:HG3	1:A:61:ALA:HA	2	0.04	0.04
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	2	0.01	0.02
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE22	2	0.01	0.02
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	2	0.01	0.02
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE22	2	0.01	0.02
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	2	0.01	0.02
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE22	2	0.01	0.02
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	2	0.01	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	2	0.01	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	2	0.01	0.01
(1,745)	1:A:53:THR:HB	1:A:54:THR:H	2	0.04	0.04
(1,714)	1:A:50:MET:H	1:A:50:MET:HE1	2	0.01	0.02
(1,714)	1:A:50:MET:H	1:A:50:MET:HE2	2	0.01	0.02
(1,714)	1:A:50:MET:H	1:A:50:MET:HE3	2	0.01	0.02
(1,708)	1:A:50:MET:HE1	1:A:55:ALA:H	2	0.04	0.06
(1,708)	1:A:50:MET:HE2	1:A:55:ALA:H	2	0.04	0.06

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,708)	1:A:50:MET:HE3	1:A:55:ALA:H	2	0.04	0.06
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB1	2	0.06	0.08
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB2	2	0.06	0.08
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB3	2	0.06	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB1	2	0.06	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB2	2	0.06	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB3	2	0.06	0.08
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	2	0.04	0.04
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	2	0.04	0.04
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	2	0.04	0.04
(1,67)	1:B:11:LEU:HD21	1:A:98:ASP:H	2	0.04	0.04
(1,67)	1:B:11:LEU:HD22	1:A:98:ASP:H	2	0.04	0.04
(1,67)	1:B:11:LEU:HD23	1:A:98:ASP:H	2	0.04	0.04
(1,66)	1:B:11:LEU:HD11	1:A:98:ASP:HB2	2	0.06	0.1
(1,66)	1:B:11:LEU:HD12	1:A:98:ASP:HB2	2	0.06	0.1
(1,66)	1:B:11:LEU:HD13	1:A:98:ASP:HB2	2	0.06	0.1
(1,66)	1:B:11:LEU:HD21	1:A:98:ASP:HB2	2	0.06	0.1
(1,66)	1:B:11:LEU:HD22	1:A:98:ASP:HB2	2	0.06	0.1
(1,66)	1:B:11:LEU:HD23	1:A:98:ASP:HB2	2	0.06	0.1
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	2	0.03	0.03
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	2	0.03	0.03
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	2	0.03	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	2	0.03	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	2	0.03	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	2	0.03	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	2	0.03	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	2	0.03	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	2	0.03	0.03
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	2	0.03	0.05
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	2	0.03	0.05
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	2	0.03	0.05
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	2	0.02	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	2	0.02	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	2	0.02	0.02
(1,613)	1:A:42:GLU:HG2	1:A:52:LEU:HG	2	0.04	0.04
(1,613)	1:A:42:GLU:HG3	1:A:52:LEU:HG	2	0.04	0.04
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	2	0.03	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	2	0.03	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	2	0.03	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD11	2	0.03	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD12	2	0.03	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD13	2	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,522)	1:A:38:GLU:HG2	1:A:39:ARG:H	2	0.07	0.07
(1,522)	1:A:38:GLU:HG3	1:A:39:ARG:H	2	0.07	0.07
(1,520)	1:A:38:GLU:HB2	1:A:80:ARG:HE	2	0.07	0.11
(1,520)	1:A:38:GLU:HB3	1:A:80:ARG:HE	2	0.07	0.11
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE21	2	0.03	0.04
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE22	2	0.03	0.04
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	2	0.07	0.07
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	2	0.07	0.07
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	2	0.07	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	2	0.07	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	2	0.07	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	2	0.07	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	2	0.07	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	2	0.07	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	2	0.07	0.07
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	2	0.03	0.03
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	2	0.03	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	2	0.03	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	2	0.03	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	2	0.03	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	2	0.03	0.03
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD11	2	0.09	0.11
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD12	2	0.09	0.11
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD13	2	0.09	0.11
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	2	0.02	0.02
(1,360)	1:A:29:GLN:HG3	1:A:48:THR:HB	2	0.02	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	2	0.01	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	2	0.01	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	2	0.01	0.02
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	2	0.04	0.06
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	2	0.03	0.04
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	2	0.03	0.04
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	2	0.03	0.04
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	2	0.02	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	2	0.02	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	2	0.02	0.03
(1,278)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	2	0.03	0.05
(1,278)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	2	0.03	0.05
(1,278)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	2	0.03	0.05
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	2	0.03	0.04
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	2	0.03	0.04
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	2	0.03	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD11	2	0.03	0.04
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD12	2	0.03	0.04
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD13	2	0.03	0.04
(1,2595)	1:B:91:ALA:H	1:B:87:ALA:O	2	0.02	0.02
(1,2579)	1:B:78:TYR:H	1:B:71:ARG:O	2	0.02	0.02
(1,2575)	1:B:73:GLU:H	1:B:76:ARG:O	2	0.02	0.02
(1,2569)	1:B:67:LEU:H	1:B:62:LEU:O	2	0.03	0.03
(1,2555)	1:B:60:GLN:H	1:B:56:SER:O	2	0.01	0.02
(1,2539)	1:B:48:THR:H	1:B:44:ILE:O	2	0.01	0.01
(1,2519)	1:B:32:ASP:H	1:B:28:LEU:O	2	0.03	0.03
(1,2511)	1:B:19:GLY:H	1:B:15:VAL:O	2	0.01	0.01
(1,2454)	1:A:66:GLY:N	1:A:63:LYS:O	2	0.06	0.06
(1,2425)	1:A:48:THR:H	1:A:44:ILE:O	2	0.01	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	2	0.01	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	2	0.01	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	2	0.01	0.02
(1,2391)	1:A:16:ALA:H	1:A:12:LEU:O	2	0.01	0.01
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	2	0.02	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	2	0.02	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	2	0.02	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG11	2	0.02	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG12	2	0.02	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG13	2	0.02	0.02
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG11	2	0.05	0.06
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG12	2	0.05	0.06
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG13	2	0.05	0.06
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	2	0.08	0.14
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	2	0.08	0.14
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	2	0.08	0.14
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	2	0.08	0.14
(1,2191)	1:B:81:ILE:HG21	1:B:83:GLY:H	2	0.04	0.04
(1,2191)	1:B:81:ILE:HG22	1:B:83:GLY:H	2	0.04	0.04
(1,2191)	1:B:81:ILE:HG23	1:B:83:GLY:H	2	0.04	0.04
(1,2179)	1:B:81:ILE:HD11	1:B:82:ALA:H	2	0.02	0.02
(1,2179)	1:B:81:ILE:HD12	1:B:82:ALA:H	2	0.02	0.02
(1,2179)	1:B:81:ILE:HD13	1:B:82:ALA:H	2	0.02	0.02
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG2	2	0.03	0.03
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG3	2	0.03	0.03
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	2	0.03	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE2	2	0.03	0.05
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE1	2	0.03	0.05
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE2	2	0.03	0.05
(1,2152)	1:B:76:ARG:H	1:B:76:ARG:HG2	2	0.11	0.15
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	2	0.04	0.05
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE2	2	0.04	0.05
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	2	0.04	0.05
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE2	2	0.04	0.05
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	2	0.05	0.08
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB3	2	0.05	0.08
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB2	2	0.05	0.08
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB3	2	0.05	0.08
(1,2086)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	2	0.04	0.05
(1,2086)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	2	0.04	0.05
(1,2086)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	2	0.04	0.05
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	2	0.01	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	2	0.01	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	2	0.01	0.01
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	2	0.05	0.07
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	2	0.05	0.07
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	2	0.07	0.12
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	2	0.07	0.12
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	2	0.07	0.12
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	2	0.07	0.12
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	2	0.07	0.12
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	2	0.07	0.12
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG11	2	0.03	0.04
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG12	2	0.03	0.04
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG13	2	0.03	0.04
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	2	0.02	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	2	0.02	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	2	0.02	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	2	0.02	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	2	0.02	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	2	0.02	0.02
(1,1986)	1:B:63:LYS:HB2	1:B:69:GLU:HA	2	0.03	0.04
(1,1986)	1:B:63:LYS:HB3	1:B:69:GLU:HA	2	0.03	0.04
(1,1951)	1:B:60:GLN:HG2	1:B:61:ALA:HA	2	0.03	0.03
(1,1951)	1:B:60:GLN:HG3	1:B:61:ALA:HA	2	0.03	0.03
(1,1874)	1:B:53:THR:HB	1:B:54:THR:H	2	0.04	0.08
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB1	2	0.01	0.02
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB2	2	0.01	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB3	2	0.01	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB1	2	0.01	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB2	2	0.01	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB3	2	0.01	0.02
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	2	0.06	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	2	0.06	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	2	0.06	0.07
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG2	2	0.02	0.02
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG3	2	0.02	0.02
(1,1620)	1:B:34:LEU:HD21	1:B:80:ARG:HA	2	0.01	0.02
(1,1620)	1:B:34:LEU:HD22	1:B:80:ARG:HA	2	0.01	0.02
(1,1620)	1:B:34:LEU:HD23	1:B:80:ARG:HA	2	0.01	0.02
(1,1616)	1:B:34:LEU:HD11	1:B:80:ARG:HA	2	0.02	0.03
(1,1616)	1:B:34:LEU:HD12	1:B:80:ARG:HA	2	0.02	0.03
(1,1616)	1:B:34:LEU:HD13	1:B:80:ARG:HA	2	0.02	0.03
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	2	0.07	0.12
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	2	0.07	0.12
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	2	0.04	0.05
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	2	0.04	0.05
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	2	0.04	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD21	2	0.04	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD22	2	0.04	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD23	2	0.04	0.05
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	2	0.08	0.1
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB3	2	0.08	0.1
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB2	2	0.08	0.1
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB3	2	0.08	0.1
(1,1437)	1:B:23:ALA:H	1:B:24:ASN:H	2	0.16	0.28
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	2	0.01	0.01
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	2	0.01	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	2	0.01	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	2	0.01	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	2	0.01	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	2	0.01	0.01
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	2	0.03	0.04
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	2	0.03	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	2	0.03	0.04
(1,1424)	1:B:22:LEU:HD11	1:B:93:VAL:HB	2	0.04	0.05
(1,1424)	1:B:22:LEU:HD12	1:B:93:VAL:HB	2	0.04	0.05
(1,1424)	1:B:22:LEU:HD13	1:B:93:VAL:HB	2	0.04	0.05
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD21	2	0.04	0.05
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD22	2	0.04	0.05
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD23	2	0.04	0.05
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	2	0.01	0.01
(1,141)	1:A:7:ARG:HB3	1:A:8:LYS:H	2	0.01	0.01
(1,1407)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	2	0.03	0.04
(1,1407)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	2	0.03	0.04
(1,1407)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	2	0.03	0.04
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	2	0.04	0.04
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	2	0.04	0.04
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	2	0.04	0.04
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	2	0.04	0.04
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE2	2	0.04	0.04
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE3	2	0.04	0.04
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	2	0.03	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	2	0.03	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	2	0.03	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD11	2	0.04	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD12	2	0.04	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD13	2	0.04	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD21	2	0.04	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD22	2	0.04	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD23	2	0.04	0.06
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	2	0.03	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	2	0.03	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	2	0.03	0.03
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG11	2	0.08	0.08
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG12	2	0.08	0.08
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG13	2	0.08	0.08
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	2	0.04	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	2	0.04	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	2	0.04	0.05
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	2	0.02	0.03
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	2	0.02	0.03
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	2	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG11	2	0.02	0.03
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG12	2	0.02	0.03
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG13	2	0.02	0.03
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG11	2	0.06	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG12	2	0.06	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG13	2	0.06	0.06
(1,1141)	1:A:89:LEU:HD21	1:A:93:VAL:HB	2	0.02	0.02
(1,1141)	1:A:89:LEU:HD22	1:A:93:VAL:HB	2	0.02	0.02
(1,1141)	1:A:89:LEU:HD23	1:A:93:VAL:HB	2	0.02	0.02
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	2	0.05	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	2	0.05	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	2	0.05	0.07
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD2	2	0.03	0.03
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD3	2	0.03	0.03
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	2	0.02	0.03
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE2	2	0.02	0.03
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	2	0.02	0.03
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE2	2	0.02	0.03
(1,994)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	1	0.07	0.07
(1,994)	1:A:73:GLU:HG2	1:A:78:TYR:HD2	1	0.07	0.07
(1,994)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	1	0.07	0.07
(1,994)	1:A:73:GLU:HG3	1:A:78:TYR:HD2	1	0.07	0.07
(1,988)	1:A:72:ARG:H	1:A:72:ARG:HD2	1	0.09	0.09
(1,988)	1:A:72:ARG:H	1:A:72:ARG:HD3	1	0.09	0.09
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD13	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD13	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD13	1	0.05	0.05
(1,978)	1:A:72:ARG:HA	1:A:77:GLN:HA	1	0.01	0.01
(1,974)	1:A:72:ARG:HA	1:A:72:ARG:HD2	1	0.05	0.05
(1,974)	1:A:72:ARG:HA	1:A:72:ARG:HD3	1	0.05	0.05
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD11	1	0.01	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD12	1	0.01	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD13	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,965)	1:A:71:ARG:HB2	1:A:71:ARG:HE	1	0.02	0.02
(1,965)	1:A:71:ARG:HB3	1:A:71:ARG:HE	1	0.02	0.02
(1,957)	1:A:70:ALA:HB1	1:A:77:GLN:HE22	1	0.03	0.03
(1,957)	1:A:70:ALA:HB2	1:A:77:GLN:HE22	1	0.03	0.03
(1,957)	1:A:70:ALA:HB3	1:A:77:GLN:HE22	1	0.03	0.03
(1,956)	1:A:70:ALA:HB1	1:A:77:GLN:HE21	1	0.02	0.02
(1,956)	1:A:70:ALA:HB2	1:A:77:GLN:HE21	1	0.02	0.02
(1,956)	1:A:70:ALA:HB3	1:A:77:GLN:HE21	1	0.02	0.02
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB1	1	0.05	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB2	1	0.05	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB3	1	0.05	0.05
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG11	1	0.03	0.03
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG12	1	0.03	0.03
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG13	1	0.03	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG11	1	0.03	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG12	1	0.03	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG13	1	0.03	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG11	1	0.03	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG12	1	0.03	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG13	1	0.03	0.03
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD21	1	0.02	0.02
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD22	1	0.02	0.02
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD23	1	0.02	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD21	1	0.02	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD22	1	0.02	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD23	1	0.02	0.02
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD21	1	0.09	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD22	1	0.09	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD23	1	0.09	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD21	1	0.09	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD22	1	0.09	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD23	1	0.09	0.09
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD11	1	0.02	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD12	1	0.02	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD13	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD11	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD12	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD13	1	0.02	0.02
(1,879)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	1	0.06	0.06
(1,879)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	1	0.06	0.06
(1,879)	1:A:65:GLY:HA3	1:A:67:LEU:HB2	1	0.06	0.06
(1,879)	1:A:65:GLY:HA3	1:A:67:LEU:HB3	1	0.06	0.06

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,870)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	1	0.05	0.05
(1,870)	1:A:63:LYS:HG2	1:A:79:TYR:HE2	1	0.05	0.05
(1,870)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	1	0.05	0.05
(1,870)	1:A:63:LYS:HG3	1:A:79:TYR:HE2	1	0.05	0.05
(1,857)	1:A:63:LYS:HB2	1:A:69:GLU:HA	1	0.11	0.11
(1,857)	1:A:63:LYS:HB3	1:A:69:GLU:HA	1	0.11	0.11
(1,852)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	1	0.01	0.01
(1,852)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	1	0.01	0.01
(1,852)	1:A:63:LYS:HB3	1:A:63:LYS:HE2	1	0.01	0.01
(1,852)	1:A:63:LYS:HB3	1:A:63:LYS:HE3	1	0.01	0.01
(1,846)	1:A:62:LEU:H	1:A:62:LEU:HG	1	0.17	0.17
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG21	1	0.03	0.03
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG22	1	0.03	0.03
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG23	1	0.03	0.03
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD11	1	0.08	0.08
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD12	1	0.08	0.08
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD13	1	0.08	0.08
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD11	1	0.01	0.01
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD12	1	0.01	0.01
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD13	1	0.01	0.01
(1,76)	1:B:12:LEU:HD21	1:A:28:LEU:HB2	1	0.01	0.01
(1,76)	1:B:12:LEU:HD21	1:A:28:LEU:HB3	1	0.01	0.01
(1,76)	1:B:12:LEU:HD22	1:A:28:LEU:HB2	1	0.01	0.01
(1,76)	1:B:12:LEU:HD22	1:A:28:LEU:HB3	1	0.01	0.01
(1,76)	1:B:12:LEU:HD23	1:A:28:LEU:HB2	1	0.01	0.01
(1,76)	1:B:12:LEU:HD23	1:A:28:LEU:HB3	1	0.01	0.01
(1,748)	1:A:53:THR:H	1:A:53:THR:HB	1	0.01	0.01
(1,746)	1:A:53:THR:HB	1:A:55:ALA:H	1	0.01	0.01
(1,740)	1:A:52:LEU:HD11	1:A:56:SER:H	1	0.02	0.02
(1,740)	1:A:52:LEU:HD12	1:A:56:SER:H	1	0.02	0.02
(1,740)	1:A:52:LEU:HD13	1:A:56:SER:H	1	0.02	0.02
(1,740)	1:A:52:LEU:HD21	1:A:56:SER:H	1	0.02	0.02
(1,740)	1:A:52:LEU:HD22	1:A:56:SER:H	1	0.02	0.02
(1,740)	1:A:52:LEU:HD23	1:A:56:SER:H	1	0.02	0.02
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	1	0.04	0.04
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	1	0.04	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	1	0.04	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	1	0.04	0.04
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	1	0.04	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	1	0.04	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB2	1	0.04	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB3	1	0.04	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB2	1	0.04	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB3	1	0.04	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB1	1	0.04	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB2	1	0.04	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB3	1	0.04	0.04
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG21	1	0.01	0.01
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG22	1	0.01	0.01
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG23	1	0.01	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG21	1	0.01	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG22	1	0.01	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG23	1	0.01	0.01
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD21	1	0.02	0.02
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD22	1	0.02	0.02
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD23	1	0.02	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD21	1	0.02	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD22	1	0.02	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD23	1	0.02	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD21	1	0.02	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD22	1	0.02	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD23	1	0.02	0.02
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	1	0.04	0.04
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	1	0.04	0.04
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	1	0.04	0.04
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD11	1	0.03	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD12	1	0.03	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD13	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD11	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD12	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD13	1	0.03	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	1	0.03	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	1	0.03	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	1	0.03	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD21	1	0.03	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD22	1	0.03	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD23	1	0.03	0.03
(1,572)	1:A:41:VAL:HB	1:A:79:TYR:HE1	1	0.02	0.02
(1,572)	1:A:41:VAL:HB	1:A:79:TYR:HE2	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,547)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	1	0.02	0.02
(1,547)	1:A:40:ALA:HB1	1:A:42:GLU:HG3	1	0.02	0.02
(1,547)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	1	0.02	0.02
(1,547)	1:A:40:ALA:HB2	1:A:42:GLU:HG3	1	0.02	0.02
(1,547)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	1	0.02	0.02
(1,547)	1:A:40:ALA:HB3	1:A:42:GLU:HG3	1	0.02	0.02
(1,532)	1:A:39:ARG:HB2	1:A:39:ARG:HE	1	0.04	0.04
(1,532)	1:A:39:ARG:HB3	1:A:39:ARG:HE	1	0.04	0.04
(1,523)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	1	0.04	0.04
(1,523)	1:A:38:GLU:HG2	1:A:78:TYR:HB3	1	0.04	0.04
(1,523)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	1	0.04	0.04
(1,523)	1:A:38:GLU:HG3	1:A:78:TYR:HB3	1	0.04	0.04
(1,511)	1:A:36:GLN:HG2	1:A:37:GLY:H	1	0.02	0.02
(1,511)	1:A:36:GLN:HG3	1:A:37:GLY:H	1	0.02	0.02
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB1	1	0.04	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB2	1	0.04	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB3	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB1	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB2	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB3	1	0.04	0.04
(1,504)	1:A:35:ALA:HB1	1:A:90:PHE:HD1	1	0.03	0.03
(1,504)	1:A:35:ALA:HB1	1:A:90:PHE:HD2	1	0.03	0.03
(1,504)	1:A:35:ALA:HB2	1:A:90:PHE:HD1	1	0.03	0.03
(1,504)	1:A:35:ALA:HB2	1:A:90:PHE:HD2	1	0.03	0.03
(1,504)	1:A:35:ALA:HB3	1:A:90:PHE:HD1	1	0.03	0.03
(1,504)	1:A:35:ALA:HB3	1:A:90:PHE:HD2	1	0.03	0.03
(1,500)	1:A:35:ALA:HB1	1:A:36:GLN:HE21	1	0.13	0.13
(1,500)	1:A:35:ALA:HB1	1:A:36:GLN:HE22	1	0.13	0.13
(1,500)	1:A:35:ALA:HB2	1:A:36:GLN:HE21	1	0.13	0.13
(1,500)	1:A:35:ALA:HB2	1:A:36:GLN:HE22	1	0.13	0.13
(1,500)	1:A:35:ALA:HB3	1:A:36:GLN:HE21	1	0.13	0.13
(1,500)	1:A:35:ALA:HB3	1:A:36:GLN:HE22	1	0.13	0.13
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB1	1	0.07	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB2	1	0.07	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB3	1	0.07	0.07
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD11	1	0.01	0.01
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD12	1	0.01	0.01
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD13	1	0.01	0.01
(1,488)	1:A:34:LEU:HD21	1:A:37:GLY:H	1	0.01	0.01
(1,488)	1:A:34:LEU:HD22	1:A:37:GLY:H	1	0.01	0.01
(1,488)	1:A:34:LEU:HD23	1:A:37:GLY:H	1	0.01	0.01
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	1	0.04	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	1	0.04	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	1	0.04	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	1	0.04	0.04
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	1	0.04	0.04
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	1	0.04	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB1	1	0.04	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB3	1	0.04	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB1	1	0.04	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB3	1	0.04	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB1	1	0.04	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB2	1	0.04	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB3	1	0.04	0.04
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD11	1	0.01	0.01
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD12	1	0.01	0.01
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD13	1	0.01	0.01
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG11	1	0.02	0.02
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG12	1	0.02	0.02
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG13	1	0.02	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG11	1	0.02	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG12	1	0.02	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG13	1	0.02	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG11	1	0.02	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG12	1	0.02	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG13	1	0.02	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD11	1	0.02	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD12	1	0.02	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD13	1	0.02	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD11	1	0.02	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD12	1	0.02	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD13	1	0.02	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD11	1	0.02	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD12	1	0.02	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD13	1	0.02	0.02
(1,433)	1:A:31:LEU:HD21	1:A:81:ILE:HA	1	0.01	0.01
(1,433)	1:A:31:LEU:HD22	1:A:81:ILE:HA	1	0.01	0.01
(1,433)	1:A:31:LEU:HD23	1:A:81:ILE:HA	1	0.01	0.01
(1,428)	1:A:31:LEU:HD21	1:A:67:LEU:HA	1	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,428)	1:A:31:LEU:HD22	1:A:67:LEU:HA	1	0.03	0.03
(1,428)	1:A:31:LEU:HD23	1:A:67:LEU:HA	1	0.03	0.03
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG11	1	0.01	0.01
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG12	1	0.01	0.01
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG13	1	0.01	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG11	1	0.01	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG12	1	0.01	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG13	1	0.01	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG11	1	0.01	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG12	1	0.01	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG13	1	0.01	0.01
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HG	1	0.05	0.05
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HG	1	0.05	0.05
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HG	1	0.05	0.05
(1,381)	1:A:30:ILE:HD11	1:A:59:LEU:HA	1	0.02	0.02
(1,381)	1:A:30:ILE:HD12	1:A:59:LEU:HA	1	0.02	0.02
(1,381)	1:A:30:ILE:HD13	1:A:59:LEU:HA	1	0.02	0.02
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD11	1	0.01	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD12	1	0.01	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD13	1	0.01	0.01
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE1	1	0.01	0.01
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE2	1	0.01	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE1	1	0.01	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE2	1	0.01	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE1	1	0.01	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE2	1	0.01	0.01
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE1	1	0.02	0.02
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE2	1	0.02	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE1	1	0.02	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE2	1	0.02	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE1	1	0.02	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE2	1	0.02	0.02
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	1	0.04	0.04
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	1	0.04	0.04
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	1	0.04	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB1	1	0.04	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB2	1	0.04	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB3	1	0.04	0.04
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG2	1	0.11	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG3	1	0.11	0.11
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD11	1	0.08	0.08
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD12	1	0.08	0.08

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD13	1	0.08	0.08
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG13	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG13	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG13	1	0.02	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD21	1	0.02	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD22	1	0.02	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD23	1	0.02	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD21	1	0.02	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD22	1	0.02	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD23	1	0.02	0.02
(1,277)	1:A:21:ALA:HB1	1:A:65:GLY:HA3	1	0.01	0.01
(1,277)	1:A:21:ALA:HB2	1:A:65:GLY:HA3	1	0.01	0.01
(1,277)	1:A:21:ALA:HB3	1:A:65:GLY:HA3	1	0.01	0.01
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD2	1	0.02	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD3	1	0.02	0.02
(1,2611)	1:B:99:GLU:H	1:B:95:VAL:O	1	0.02	0.02
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE2	1	0.03	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE3	1	0.03	0.03
(1,2568)	1:B:66:GLY:N	1:B:63:LYS:O	1	0.06	0.06
(1,2561)	1:B:63:LYS:H	1:B:59:LEU:O	1	0.01	0.01
(1,2559)	1:B:62:LEU:H	1:B:58:ASN:O	1	0.01	0.01
(1,2543)	1:B:50:MET:H	1:B:45:ALA:O	1	0.01	0.01
(1,2535)	1:B:46:THR:H	1:B:42:GLU:O	1	0.01	0.01
(1,2528)	1:B:39:ARG:N	1:B:79:TYR:O	1	0.01	0.01
(1,2510)	1:B:18:VAL:N	1:B:14:GLN:O	1	0.02	0.02
(1,2502)	1:B:14:GLN:N	1:B:10:ALA:O	1	0.01	0.01
(1,2495)	1:A:98:ASP:H	1:A:94:GLN:O	1	0.01	0.01
(1,2489)	1:A:95:VAL:H	1:A:91:ALA:O	1	0.03	0.03
(1,2479)	1:A:90:PHE:H	1:A:86:VAL:O	1	0.01	0.01
(1,2465)	1:A:78:TYR:H	1:A:71:ARG:O	1	0.01	0.01
(1,2456)	1:A:67:LEU:N	1:A:62:LEU:O	1	0.01	0.01
(1,2445)	1:A:62:LEU:H	1:A:58:ASN:O	1	0.01	0.01
(1,2429)	1:A:50:MET:H	1:A:45:ALA:O	1	0.01	0.01
(1,2405)	1:A:32:ASP:H	1:A:28:LEU:O	1	0.02	0.02
(1,2399)	1:A:20:LYS:H	1:A:16:ALA:O	1	0.01	0.01
(1,2397)	1:A:19:GLY:H	1:A:15:VAL:O	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2383)	1:B:102:GLU:H	1:B:102:GLU:HG2	1	0.02	0.02
(1,2383)	1:B:102:GLU:H	1:B:102:GLU:HG3	1	0.02	0.02
(1,2382)	1:B:101:LEU:H	1:B:102:GLU:H	1	0.18	0.18
(1,2373)	1:B:100:HIS:H	1:B:100:HIS:HD2	1	0.01	0.01
(1,2350)	1:B:96:VAL:HG21	1:B:97:ALA:H	1	0.01	0.01
(1,2350)	1:B:96:VAL:HG22	1:B:97:ALA:H	1	0.01	0.01
(1,2350)	1:B:96:VAL:HG23	1:B:97:ALA:H	1	0.01	0.01
(1,2346)	1:B:96:VAL:HA	1:B:100:HIS:HD2	1	0.14	0.14
(1,2345)	1:B:96:VAL:HA	1:B:99:GLU:HB2	1	0.05	0.05
(1,2345)	1:B:96:VAL:HA	1:B:99:GLU:HB3	1	0.05	0.05
(1,2327)	1:B:95:VAL:HA	1:B:98:ASP:HB2	1	0.03	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD2	1	0.03	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD3	1	0.03	0.03
(1,2292)	1:B:91:ALA:HA	1:B:94:GLN:HG2	1	0.02	0.02
(1,2292)	1:B:91:ALA:HA	1:B:94:GLN:HG3	1	0.02	0.02
(1,2290)	1:B:91:ALA:HA	1:B:94:GLN:HE21	1	0.05	0.05
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG11	1	0.02	0.02
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG12	1	0.02	0.02
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG13	1	0.02	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG11	1	0.02	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG12	1	0.02	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG13	1	0.02	0.02
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG11	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG12	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG13	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG11	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG12	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG13	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG11	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG12	1	0.01	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG13	1	0.01	0.01
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG21	1	0.03	0.03
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG22	1	0.03	0.03
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG23	1	0.03	0.03
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB1	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB2	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB3	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB1	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB2	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB3	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB1	1	0.02	0.02
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB2	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB3	1	0.02	0.02
(1,2151)	1:B:76:ARG:H	1:B:76:ARG:HG3	1	0.18	0.18
(1,2148)	1:B:76:ARG:HG2	1:B:77:GLN:H	1	0.05	0.05
(1,2148)	1:B:76:ARG:HG3	1:B:77:GLN:H	1	0.05	0.05
(1,2124)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	1	0.01	0.01
(1,2124)	1:B:73:GLU:HG2	1:B:78:TYR:HE2	1	0.01	0.01
(1,2124)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	1	0.01	0.01
(1,2124)	1:B:73:GLU:HG3	1:B:78:TYR:HE2	1	0.01	0.01
(1,2123)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	1	0.03	0.03
(1,2123)	1:B:73:GLU:HG2	1:B:78:TYR:HD2	1	0.03	0.03
(1,2123)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	1	0.03	0.03
(1,2123)	1:B:73:GLU:HG3	1:B:78:TYR:HD2	1	0.03	0.03
(1,2121)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	1	0.11	0.11
(1,2121)	1:B:73:GLU:HB2	1:B:78:TYR:HD2	1	0.11	0.11
(1,2121)	1:B:73:GLU:HB3	1:B:78:TYR:HD1	1	0.11	0.11
(1,2121)	1:B:73:GLU:HB3	1:B:78:TYR:HD2	1	0.11	0.11
(1,210)	1:A:15:VAL:HA	1:A:18:VAL:HB	1	0.02	0.02
(1,2096)	1:B:71:ARG:HB2	1:B:79:TYR:HA	1	0.03	0.03
(1,2096)	1:B:71:ARG:HB3	1:B:79:TYR:HA	1	0.03	0.03
(1,2085)	1:B:70:ALA:HB1	1:B:77:GLN:HE21	1	0.01	0.01
(1,2085)	1:B:70:ALA:HB2	1:B:77:GLN:HE21	1	0.01	0.01
(1,2085)	1:B:70:ALA:HB3	1:B:77:GLN:HE21	1	0.01	0.01
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB1	1	0.02	0.02
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB2	1	0.02	0.02
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB3	1	0.02	0.02
(1,2072)	1:B:69:GLU:HG2	1:B:82:ALA:HA	1	0.05	0.05
(1,2070)	1:B:69:GLU:HG3	1:B:82:ALA:HA	1	0.05	0.05
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG11	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG12	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG13	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG11	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG12	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG13	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG11	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG12	1	0.01	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG13	1	0.01	0.01
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD21	1	0.03	0.03
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD22	1	0.03	0.03
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD23	1	0.03	0.03
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG11	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG12	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG13	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG11	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG12	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG13	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG11	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG12	1	0.01	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG13	1	0.01	0.01
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD11	1	0.09	0.09
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD12	1	0.09	0.09
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD13	1	0.09	0.09
(1,2008)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	1	0.04	0.04
(1,2008)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	1	0.04	0.04
(1,2008)	1:B:65:GLY:HA3	1:B:67:LEU:HB2	1	0.04	0.04
(1,2008)	1:B:65:GLY:HA3	1:B:67:LEU:HB3	1	0.04	0.04
(1,1992)	1:B:63:LYS:HE2	1:B:70:ALA:H	1	0.02	0.02
(1,1992)	1:B:63:LYS:HE3	1:B:70:ALA:H	1	0.02	0.02
(1,1990)	1:B:63:LYS:HE2	1:B:69:GLU:HA	1	0.01	0.01
(1,1990)	1:B:63:LYS:HE3	1:B:69:GLU:HA	1	0.01	0.01
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	1	0.28	0.28
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	1	0.28	0.28
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	1	0.28	0.28
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD21	1	0.28	0.28
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD22	1	0.28	0.28
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD23	1	0.28	0.28
(1,1943)	1:B:60:GLN:HA	1:B:60:GLN:HE21	1	0.01	0.01
(1,1943)	1:B:60:GLN:HA	1:B:60:GLN:HE22	1	0.01	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD11	1	0.01	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD12	1	0.01	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD13	1	0.01	0.01
(1,1884)	1:B:54:THR:HG21	1:B:58:ASN:HD22	1	0.03	0.03
(1,1884)	1:B:54:THR:HG22	1:B:58:ASN:HD22	1	0.03	0.03
(1,1884)	1:B:54:THR:HG23	1:B:58:ASN:HD22	1	0.03	0.03
(1,1882)	1:B:54:THR:HG21	1:B:57:ALA:H	1	0.04	0.04
(1,1882)	1:B:54:THR:HG22	1:B:57:ALA:H	1	0.04	0.04
(1,1882)	1:B:54:THR:HG23	1:B:57:ALA:H	1	0.04	0.04
(1,1877)	1:B:53:THR:H	1:B:53:THR:HB	1	0.01	0.01
(1,1872)	1:B:52:LEU:H	1:B:52:LEU:HG	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD11	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD11	1:B:56:SER:HB3	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD12	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD12	1:B:56:SER:HB3	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD13	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD13	1:B:56:SER:HB3	1	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1868)	1:B:52:LEU:HD21	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD21	1:B:56:SER:HB3	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD22	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD22	1:B:56:SER:HB3	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD23	1:B:56:SER:HB2	1	0.03	0.03
(1,1868)	1:B:52:LEU:HD23	1:B:56:SER:HB3	1	0.03	0.03
(1,1844)	1:B:50:MET:H	1:B:50:MET:HG2	1	0.13	0.13
(1,1844)	1:B:50:MET:H	1:B:50:MET:HG3	1	0.13	0.13
(1,1832)	1:B:50:MET:HB2	1:B:55:ALA:H	1	0.03	0.03
(1,1832)	1:B:50:MET:HB3	1:B:55:ALA:H	1	0.03	0.03
(1,1818)	1:B:48:THR:HB	1:B:50:MET:HG2	1	0.06	0.06
(1,1818)	1:B:48:THR:HB	1:B:50:MET:HG3	1	0.06	0.06
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE1	1	0.02	0.02
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE2	1	0.02	0.02
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE3	1	0.02	0.02
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	1	0.01	0.01
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	1	0.01	0.01
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	1	0.01	0.01
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	1	0.03	0.03
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	1	0.03	0.03
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	1	0.03	0.03
(1,1723)	1:B:41:VAL:HG21	1:B:79:TYR:HE1	1	0.01	0.01
(1,1723)	1:B:41:VAL:HG21	1:B:79:TYR:HE2	1	0.01	0.01
(1,1723)	1:B:41:VAL:HG22	1:B:79:TYR:HE1	1	0.01	0.01
(1,1723)	1:B:41:VAL:HG22	1:B:79:TYR:HE2	1	0.01	0.01
(1,1723)	1:B:41:VAL:HG23	1:B:79:TYR:HE1	1	0.01	0.01
(1,1723)	1:B:41:VAL:HG23	1:B:79:TYR:HE2	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG21	1:B:79:TYR:HD1	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG21	1:B:79:TYR:HD2	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG22	1:B:79:TYR:HD1	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG22	1:B:79:TYR:HD2	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG23	1:B:79:TYR:HD1	1	0.01	0.01
(1,1722)	1:B:41:VAL:HG23	1:B:79:TYR:HD2	1	0.01	0.01
(1,1683)	1:B:40:ALA:HB1	1:B:76:ARG:HD2	1	0.12	0.12
(1,1683)	1:B:40:ALA:HB1	1:B:76:ARG:HD3	1	0.12	0.12
(1,1683)	1:B:40:ALA:HB2	1:B:76:ARG:HD2	1	0.12	0.12
(1,1683)	1:B:40:ALA:HB2	1:B:76:ARG:HD3	1	0.12	0.12
(1,1683)	1:B:40:ALA:HB3	1:B:76:ARG:HD2	1	0.12	0.12
(1,1683)	1:B:40:ALA:HB3	1:B:76:ARG:HD3	1	0.12	0.12
(1,1676)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	1	0.01	0.01
(1,1676)	1:B:40:ALA:HB1	1:B:42:GLU:HG3	1	0.01	0.01
(1,1676)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1676)	1:B:40:ALA:HB2	1:B:42:GLU:HG3	1	0.01	0.01
(1,1676)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	1	0.01	0.01
(1,1676)	1:B:40:ALA:HB3	1:B:42:GLU:HG3	1	0.01	0.01
(1,1657)	1:B:39:ARG:HA	1:B:39:ARG:HD2	1	0.01	0.01
(1,1657)	1:B:39:ARG:HA	1:B:39:ARG:HD3	1	0.01	0.01
(1,1653)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	1	0.02	0.02
(1,1653)	1:B:38:GLU:HG2	1:B:78:TYR:HD2	1	0.02	0.02
(1,1653)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	1	0.02	0.02
(1,1653)	1:B:38:GLU:HG3	1:B:78:TYR:HD2	1	0.02	0.02
(1,1651)	1:B:38:GLU:HG2	1:B:39:ARG:H	1	0.18	0.18
(1,1651)	1:B:38:GLU:HG3	1:B:39:ARG:H	1	0.18	0.18
(1,1649)	1:B:38:GLU:HB2	1:B:80:ARG:HE	1	0.05	0.05
(1,1649)	1:B:38:GLU:HB3	1:B:80:ARG:HE	1	0.05	0.05
(1,1629)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	1	0.04	0.04
(1,1629)	1:B:35:ALA:HB1	1:B:36:GLN:HE22	1	0.04	0.04
(1,1629)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	1	0.04	0.04
(1,1629)	1:B:35:ALA:HB2	1:B:36:GLN:HE22	1	0.04	0.04
(1,1629)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	1	0.04	0.04
(1,1629)	1:B:35:ALA:HB3	1:B:36:GLN:HE22	1	0.04	0.04
(1,1617)	1:B:34:LEU:HD21	1:B:37:GLY:H	1	0.04	0.04
(1,1617)	1:B:34:LEU:HD22	1:B:37:GLY:H	1	0.04	0.04
(1,1617)	1:B:34:LEU:HD23	1:B:37:GLY:H	1	0.04	0.04
(1,1602)	1:B:33:LEU:HG	1:B:36:GLN:HE21	1	0.05	0.05
(1,1602)	1:B:33:LEU:HG	1:B:36:GLN:HE22	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD11	1:B:36:GLN:HG3	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD12	1:B:36:GLN:HG3	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD13	1:B:36:GLN:HG3	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD21	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD21	1:B:36:GLN:HG3	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD22	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD22	1:B:36:GLN:HG3	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD23	1:B:36:GLN:HG2	1	0.05	0.05
(1,1592)	1:B:33:LEU:HD23	1:B:36:GLN:HG3	1	0.05	0.05
(1,1591)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD11	1:B:36:GLN:HE22	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD12	1:B:36:GLN:HE22	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD13	1:B:36:GLN:HE22	1	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1591)	1:B:33:LEU:HD21	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD21	1:B:36:GLN:HE22	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD22	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD22	1:B:36:GLN:HE22	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD23	1:B:36:GLN:HE21	1	0.03	0.03
(1,1591)	1:B:33:LEU:HD23	1:B:36:GLN:HE22	1	0.03	0.03
(1,1587)	1:B:33:LEU:HA	1:B:36:GLN:HE21	1	0.01	0.01
(1,1587)	1:B:33:LEU:HA	1:B:36:GLN:HE22	1	0.01	0.01
(1,1568)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	1	0.02	0.02
(1,1568)	1:B:31:LEU:HD21	1:B:90:PHE:HE2	1	0.02	0.02
(1,1568)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	1	0.02	0.02
(1,1568)	1:B:31:LEU:HD22	1:B:90:PHE:HE2	1	0.02	0.02
(1,1568)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	1	0.02	0.02
(1,1568)	1:B:31:LEU:HD23	1:B:90:PHE:HE2	1	0.02	0.02
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG11	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG12	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG13	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG11	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG12	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG13	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG11	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG12	1	0.06	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG13	1	0.06	0.06
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD11	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD12	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD13	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD11	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD12	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD13	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD11	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD12	1	0.08	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD13	1	0.08	0.08
(1,1557)	1:B:31:LEU:HD21	1:B:67:LEU:HA	1	0.05	0.05
(1,1557)	1:B:31:LEU:HD22	1:B:67:LEU:HA	1	0.05	0.05
(1,1557)	1:B:31:LEU:HD23	1:B:67:LEU:HA	1	0.05	0.05
(1,1549)	1:B:31:LEU:HD11	1:B:67:LEU:HG	1	0.01	0.01
(1,1549)	1:B:31:LEU:HD12	1:B:67:LEU:HG	1	0.01	0.01
(1,1549)	1:B:31:LEU:HD13	1:B:67:LEU:HG	1	0.01	0.01
(1,1548)	1:B:31:LEU:HD11	1:B:67:LEU:HB2	1	0.02	0.02
(1,1548)	1:B:31:LEU:HD11	1:B:67:LEU:HB3	1	0.02	0.02
(1,1548)	1:B:31:LEU:HD12	1:B:67:LEU:HB2	1	0.02	0.02
(1,1548)	1:B:31:LEU:HD12	1:B:67:LEU:HB3	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1548)	1:B:31:LEU:HD13	1:B:67:LEU:HB2	1	0.02	0.02
(1,1548)	1:B:31:LEU:HD13	1:B:67:LEU:HB3	1	0.02	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD11	1	0.02	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD12	1	0.02	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD13	1	0.02	0.02
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD11	1	0.03	0.03
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD12	1	0.03	0.03
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD13	1	0.03	0.03
(1,1509)	1:B:30:ILE:HD11	1:B:58:ASN:H	1	0.02	0.02
(1,1509)	1:B:30:ILE:HD12	1:B:58:ASN:H	1	0.02	0.02
(1,1509)	1:B:30:ILE:HD13	1:B:58:ASN:H	1	0.02	0.02
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	1	0.01	0.01
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	1	0.01	0.01
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	1	0.01	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB1	1	0.01	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB2	1	0.01	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB3	1	0.01	0.01
(1,1447)	1:B:26:ARG:HA	1:B:29:GLN:HG2	1	0.01	0.01
(1,1447)	1:B:26:ARG:HA	1:B:29:GLN:HG3	1	0.01	0.01
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD11	1	0.08	0.08
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD12	1	0.08	0.08
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD13	1	0.08	0.08
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG11	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG12	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG13	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG11	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG12	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG13	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG11	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG12	1	0.02	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG13	1	0.02	0.02
(1,1406)	1:B:21:ALA:HB1	1:B:65:GLY:HA3	1	0.05	0.05
(1,1406)	1:B:21:ALA:HB2	1:B:65:GLY:HA3	1	0.05	0.05
(1,1406)	1:B:21:ALA:HB3	1:B:65:GLY:HA3	1	0.05	0.05
(1,14)	1:A:12:LEU:HD21	1:B:28:LEU:H	1	0.02	0.02
(1,14)	1:A:12:LEU:HD22	1:B:28:LEU:H	1	0.02	0.02
(1,14)	1:A:12:LEU:HD23	1:B:28:LEU:H	1	0.02	0.02
(1,1399)	1:B:20:LYS:H	1:B:20:LYS:HD2	1	0.05	0.05
(1,1399)	1:B:20:LYS:H	1:B:20:LYS:HD3	1	0.05	0.05
(1,1374)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	1	0.06	0.06
(1,1374)	1:B:18:VAL:HG11	1:B:65:GLY:HA3	1	0.06	0.06
(1,1374)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	1	0.06	0.06

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1374)	1:B:18:VAL:HG12	1:B:65:GLY:HA3	1	0.06	0.06
(1,1374)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	1	0.06	0.06
(1,1374)	1:B:18:VAL:HG13	1:B:65:GLY:HA3	1	0.06	0.06
(1,1359)	1:B:17:ARG:H	1:B:17:ARG:HD2	1	0.02	0.02
(1,1359)	1:B:17:ARG:H	1:B:17:ARG:HD3	1	0.02	0.02
(1,1284)	1:B:8:LYS:H	1:B:8:LYS:HG2	1	0.01	0.01
(1,1284)	1:B:8:LYS:H	1:B:8:LYS:HG3	1	0.01	0.01
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB1	1	0.04	0.04
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB2	1	0.04	0.04
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB3	1	0.04	0.04
(1,1259)	1:B:5:SER:HB2	1:B:6:ASP:H	1	0.01	0.01
(1,1259)	1:B:5:SER:HB3	1:B:6:ASP:H	1	0.01	0.01
(1,1255)	1:A:107:HIS:HB2	1:A:108:HIS:H	1	0.06	0.06
(1,1255)	1:A:107:HIS:HB3	1:A:108:HIS:H	1	0.06	0.06
(1,1254)	1:A:102:GLU:H	1:A:102:GLU:HG2	1	0.07	0.07
(1,1254)	1:A:102:GLU:H	1:A:102:GLU:HG3	1	0.07	0.07
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD21	1	0.08	0.08
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD22	1	0.08	0.08
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD23	1	0.08	0.08
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD21	1	0.09	0.09
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD22	1	0.09	0.09
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD23	1	0.09	0.09
(1,1222)	1:A:96:VAL:HG21	1:A:100:HIS:HD2	1	0.1	0.1
(1,1222)	1:A:96:VAL:HG22	1:A:100:HIS:HD2	1	0.1	0.1
(1,1222)	1:A:96:VAL:HG23	1:A:100:HIS:HD2	1	0.1	0.1
(1,1220)	1:A:96:VAL:HG11	1:A:100:HIS:HD2	1	0.01	0.01
(1,1220)	1:A:96:VAL:HG12	1:A:100:HIS:HD2	1	0.01	0.01
(1,1220)	1:A:96:VAL:HG13	1:A:100:HIS:HD2	1	0.01	0.01
(1,1216)	1:A:96:VAL:HA	1:A:99:GLU:HB2	1	0.02	0.02
(1,1216)	1:A:96:VAL:HA	1:A:99:GLU:HB3	1	0.02	0.02
(1,1163)	1:A:91:ALA:HA	1:A:94:GLN:HG2	1	0.03	0.03
(1,1163)	1:A:91:ALA:HA	1:A:94:GLN:HG3	1	0.03	0.03
(1,1161)	1:A:91:ALA:HA	1:A:94:GLN:HE21	1	0.02	0.02
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB1	1	0.03	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB2	1	0.03	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB3	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB1	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB2	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB3	1	0.03	0.03
(1,1120)	1:A:87:ALA:H	1:A:88:ARG:HG2	1	0.02	0.02
(1,1120)	1:A:87:ALA:H	1:A:88:ARG:HG3	1	0.02	0.02
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB1	1	0.01	0.01

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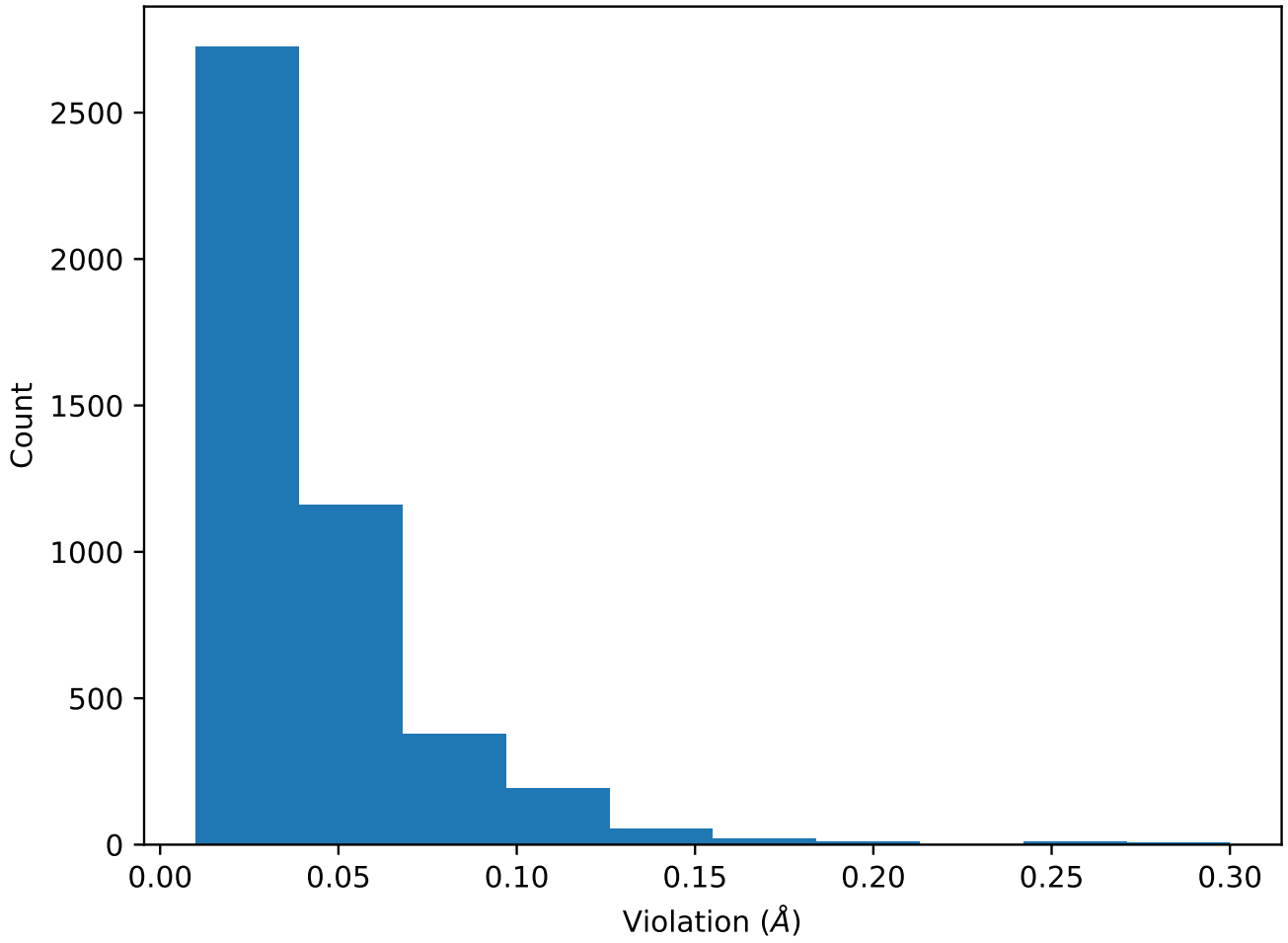
Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB2	1	0.01	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB3	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB1	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB2	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB3	1	0.01	0.01
(1,1090)	1:A:84:GLU:HG2	1:A:86:VAL:H	1	0.04	0.04
(1,1090)	1:A:84:GLU:HG3	1:A:86:VAL:H	1	0.04	0.04
(1,1076)	1:A:82:ALA:HB1	1:A:86:VAL:HB	1	0.04	0.04
(1,1076)	1:A:82:ALA:HB2	1:A:86:VAL:HB	1	0.04	0.04
(1,1076)	1:A:82:ALA:HB3	1:A:86:VAL:HB	1	0.04	0.04
(1,1075)	1:A:82:ALA:HB1	1:A:83:GLY:H	1	0.04	0.04
(1,1075)	1:A:82:ALA:HB2	1:A:83:GLY:H	1	0.04	0.04
(1,1075)	1:A:82:ALA:HB3	1:A:83:GLY:H	1	0.04	0.04
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD11	1	0.02	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD12	1	0.02	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD13	1	0.02	0.02
(1,1057)	1:A:81:ILE:HG12	1:A:87:ALA:HA	1	0.06	0.06
(1,1057)	1:A:81:ILE:HG13	1:A:87:ALA:HA	1	0.06	0.06
(1,1035)	1:A:77:GLN:H	1:A:77:GLN:HG2	1	0.01	0.01
(1,1035)	1:A:77:GLN:H	1:A:77:GLN:HG3	1	0.01	0.01
(1,1019)	1:A:76:ARG:HG2	1:A:77:GLN:H	1	0.05	0.05
(1,1019)	1:A:76:ARG:HG3	1:A:77:GLN:H	1	0.05	0.05

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)
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG2	15	0.3
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG3	15	0.3
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	3	0.28
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	3	0.28
(1,1966)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	3	0.28
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD21	3	0.28
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD22	3	0.28

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1966)	1:B:62:LEU:HB3	1:B:67:LEU:HD23	3	0.28
(1,1437)	1:B:23:ALA:H	1:B:24:ASN:H	3	0.28
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	15	0.26
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	15	0.26
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	15	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD21	15	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD22	15	0.26
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD23	15	0.26
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	14	0.25
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	14	0.25
(1,837)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	14	0.25
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD21	14	0.25
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD22	14	0.25
(1,837)	1:A:62:LEU:HB3	1:A:67:LEU:HD23	14	0.25
(1,2378)	1:B:101:LEU:HD21	1:B:102:GLU:H	14	0.21
(1,2378)	1:B:101:LEU:HD22	1:B:102:GLU:H	14	0.21
(1,2378)	1:B:101:LEU:HD23	1:B:102:GLU:H	14	0.21
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	17	0.21
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	17	0.21
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	11	0.2
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA3	11	0.2
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	11	0.2
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA3	11	0.2
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	11	0.2
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA3	11	0.2
(1,2382)	1:B:101:LEU:H	1:B:102:GLU:H	16	0.18
(1,2151)	1:B:76:ARG:H	1:B:76:ARG:HG3	12	0.18
(1,1651)	1:B:38:GLU:HG2	1:B:39:ARG:H	1	0.18
(1,1651)	1:B:38:GLU:HG3	1:B:39:ARG:H	1	0.18
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	13	0.18
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	13	0.18
(1,846)	1:A:62:LEU:H	1:A:62:LEU:HG	5	0.17
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	20	0.17
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	20	0.17
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	2	0.16
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	2	0.16
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	11	0.16
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	11	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	2	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	2	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	2	0.16
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	2	0.16

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	2	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	2	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	2	0.16
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	2	0.16
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG2	20	0.16
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG3	20	0.16
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	4	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	4	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	4	0.15
(1,2152)	1:B:76:ARG:H	1:B:76:ARG:HG2	12	0.15
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	8	0.15
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	8	0.15
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	8	0.15
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	11	0.15
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	11	0.15
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	17	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	17	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	17	0.14
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	17	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	17	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	17	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	17	0.14
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	17	0.14
(1,2346)	1:B:96:VAL:HA	1:B:100:HIS:HD2	18	0.14
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	2	0.14
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	2	0.14
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	2	0.14
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	2	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	11	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	11	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	11	0.14
(1,500)	1:A:35:ALA:HB1	1:A:36:GLN:HE21	9	0.13
(1,500)	1:A:35:ALA:HB1	1:A:36:GLN:HE22	9	0.13
(1,500)	1:A:35:ALA:HB2	1:A:36:GLN:HE21	9	0.13
(1,500)	1:A:35:ALA:HB2	1:A:36:GLN:HE22	9	0.13
(1,500)	1:A:35:ALA:HB3	1:A:36:GLN:HE21	9	0.13
(1,500)	1:A:35:ALA:HB3	1:A:36:GLN:HE22	9	0.13
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	10	0.13
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	10	0.13
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	10	0.13
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	20	0.13
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	20	0.13

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	20	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	20	0.13
(1,1844)	1:B:50:MET:H	1:B:50:MET:HG2	19	0.13
(1,1844)	1:B:50:MET:H	1:B:50:MET:HG3	19	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	8	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	8	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	8	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	19	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	19	0.13
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	13	0.13
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	13	0.13
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	13	0.13
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	4	0.13
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	4	0.13
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	4	0.13
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	3	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	3	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	3	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	3	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	3	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	3	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	3	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	3	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	5	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	5	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	5	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	5	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	5	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	5	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	5	0.12
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	5	0.12
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD11	12	0.12
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD12	12	0.12
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD13	12	0.12
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	13	0.12
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	13	0.12
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	13	0.12
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	13	0.12
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	13	0.12

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	13	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	11	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	11	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	11	0.12
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	17	0.12
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	17	0.12
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	17	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	17	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	17	0.12
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	17	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	17	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	17	0.12
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	17	0.12
(1,2270)	1:B:89:LEU:HD21	1:B:93:VAL:HB	18	0.12
(1,2270)	1:B:89:LEU:HD22	1:B:93:VAL:HB	18	0.12
(1,2270)	1:B:89:LEU:HD23	1:B:93:VAL:HB	18	0.12
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	17	0.12
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	17	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	11	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	11	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	11	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	11	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	11	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	11	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	11	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	11	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	19	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	19	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	19	0.12
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	19	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	19	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	19	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	19	0.12
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	19	0.12
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	13	0.12
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	13	0.12
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	13	0.12
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	3	0.12
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	3	0.12
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	3	0.12
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	3	0.12
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	3	0.12

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	3	0.12
(1,1683)	1:B:40:ALA:HB1	1:B:76:ARG:HD2	2	0.12
(1,1683)	1:B:40:ALA:HB1	1:B:76:ARG:HD3	2	0.12
(1,1683)	1:B:40:ALA:HB2	1:B:76:ARG:HD2	2	0.12
(1,1683)	1:B:40:ALA:HB2	1:B:76:ARG:HD3	2	0.12
(1,1683)	1:B:40:ALA:HB3	1:B:76:ARG:HD2	2	0.12
(1,1683)	1:B:40:ALA:HB3	1:B:76:ARG:HD3	2	0.12
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	4	0.12
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	4	0.12
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	20	0.12
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	20	0.12
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	20	0.12
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	6	0.11
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	6	0.11
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	6	0.11
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	6	0.11
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	6	0.11
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	6	0.11
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	6	0.11
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	6	0.11
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	4	0.11
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	4	0.11
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	4	0.11
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	11	0.11
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	11	0.11
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	11	0.11
(1,857)	1:A:63:LYS:HB2	1:A:69:GLU:HA	15	0.11
(1,857)	1:A:63:LYS:HB3	1:A:69:GLU:HA	15	0.11
(1,520)	1:A:38:GLU:HB2	1:A:80:ARG:HE	18	0.11
(1,520)	1:A:38:GLU:HB3	1:A:80:ARG:HE	18	0.11
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD11	7	0.11
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD12	7	0.11
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD13	7	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG2	6	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG3	6	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	7	0.11

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	11	0.11
(1,2121)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	19	0.11
(1,2121)	1:B:73:GLU:HB2	1:B:78:TYR:HD2	19	0.11
(1,2121)	1:B:73:GLU:HB3	1:B:78:TYR:HD1	19	0.11
(1,2121)	1:B:73:GLU:HB3	1:B:78:TYR:HD2	19	0.11
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	15	0.11
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	15	0.11
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	15	0.11
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	15	0.11
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	15	0.11
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	15	0.11
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	15	0.11
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	15	0.11
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG2	12	0.11
(1,1448)	1:B:26:ARG:H	1:B:26:ARG:HG3	12	0.11
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	7	0.11
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	7	0.11
(1,1217)	1:A:96:VAL:HA	1:A:100:HIS:HD2	15	0.11
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	7	0.1
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	7	0.1
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	7	0.1
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	7	0.1
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	7	0.1
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	7	0.1
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	7	0.1
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	7	0.1
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	14	0.1
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	14	0.1
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	14	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	14	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	14	0.1
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	14	0.1

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG2	11	0.1
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG3	11	0.1
(1,66)	1:B:11:LEU:HD11	1:A:98:ASP:HB2	2	0.1
(1,66)	1:B:11:LEU:HD12	1:A:98:ASP:HB2	2	0.1
(1,66)	1:B:11:LEU:HD13	1:A:98:ASP:HB2	2	0.1
(1,66)	1:B:11:LEU:HD21	1:A:98:ASP:HB2	2	0.1
(1,66)	1:B:11:LEU:HD22	1:A:98:ASP:HB2	2	0.1
(1,66)	1:B:11:LEU:HD23	1:A:98:ASP:HB2	2	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	19	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	19	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	19	0.1
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	18	0.1
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	18	0.1
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	18	0.1
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	19	0.1
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	19	0.1
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	19	0.1
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	3	0.1
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	14	0.1
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	15	0.1
(1,2378)	1:B:101:LEU:HD21	1:B:102:GLU:H	12	0.1
(1,2378)	1:B:101:LEU:HD22	1:B:102:GLU:H	12	0.1
(1,2378)	1:B:101:LEU:HD23	1:B:102:GLU:H	12	0.1
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	14	0.1
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	14	0.1
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	14	0.1
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	17	0.1
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	17	0.1
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	17	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	17	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	17	0.1
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	17	0.1
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	17	0.1
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB3	17	0.1
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB2	17	0.1
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB3	17	0.1
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	7	0.1
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	7	0.1
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	7	0.1
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	7	0.1
(1,1222)	1:A:96:VAL:HG21	1:A:100:HIS:HD2	17	0.1
(1,1222)	1:A:96:VAL:HG22	1:A:100:HIS:HD2	17	0.1

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1222)	1:A:96:VAL:HG23	1:A:100:HIS:HD2	17	0.1
(1,988)	1:A:72:ARG:H	1:A:72:ARG:HD2	20	0.09
(1,988)	1:A:72:ARG:H	1:A:72:ARG:HD3	20	0.09
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	18	0.09
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	18	0.09
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	18	0.09
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	18	0.09
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	18	0.09
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	18	0.09
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	18	0.09
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	18	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	3	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	3	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	3	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	8	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	8	0.09
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	8	0.09
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	15	0.09
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	15	0.09
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	15	0.09
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	15	0.09
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	15	0.09
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	15	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD21	6	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD22	6	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD23	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD21	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD22	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD23	6	0.09
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD21	14	0.09
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD22	14	0.09
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD23	14	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	9	0.09
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	15	0.09

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	15	0.09
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	15	0.09
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	16	0.09
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	16	0.09
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	16	0.09
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	11	0.09
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	11	0.09
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	20	0.09
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	20	0.09
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	17	0.09
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	17	0.09
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	19	0.09
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE2	19	0.09
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE1	19	0.09
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE2	19	0.09
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	3	0.09
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	3	0.09
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	3	0.09
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	3	0.09
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	3	0.09
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	3	0.09
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	3	0.09
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	3	0.09
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD11	6	0.09
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD12	6	0.09
(1,2015)	1:B:67:LEU:HA	1:B:67:LEU:HD13	6	0.09
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	5	0.09
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	5	0.09
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	5	0.09
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	14	0.09
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	14	0.09
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	14	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	14	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	14	0.09
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	14	0.09
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD21	16	0.09
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD22	16	0.09
(1,1227)	1:A:97:ALA:HA	1:A:101:LEU:HD23	16	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	7	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	7	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	7	0.09
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	19	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG3	19	0.08
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	19	0.08
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG3	19	0.08
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	20	0.08
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	20	0.08
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	20	0.08
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	20	0.08
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	20	0.08
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	20	0.08
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	20	0.08
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	20	0.08
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	2	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	2	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	2	0.08
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD11	5	0.08
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD12	5	0.08
(1,794)	1:A:59:LEU:HA	1:A:62:LEU:HD13	5	0.08
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB1	16	0.08
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB2	16	0.08
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB3	16	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB1	16	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB2	16	0.08
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB3	16	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	11	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	11	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	11	0.08
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	1	0.08
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	1	0.08
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	1	0.08
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	1	0.08
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD11	6	0.08
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD12	6	0.08
(1,314)	1:A:25:GLY:HA2	1:A:28:LEU:HD13	6	0.08
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	6	0.08
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB3	6	0.08
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB2	6	0.08
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB3	6	0.08
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	7	0.08
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	7	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	7	0.08
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	19	0.08
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	12	0.08
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	12	0.08
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	12	0.08
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	14	0.08
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	14	0.08
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	14	0.08
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	14	0.08
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	4	0.08
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	4	0.08
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	8	0.08
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE2	8	0.08
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE1	8	0.08
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE2	8	0.08
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	7	0.08
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB3	7	0.08
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB2	7	0.08
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB3	7	0.08
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	20	0.08
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	20	0.08
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	20	0.08
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	20	0.08
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	20	0.08
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	20	0.08
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	20	0.08
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	20	0.08
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	17	0.08
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	17	0.08
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	17	0.08
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	17	0.08
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD21	13	0.08
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD22	13	0.08
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD23	13	0.08
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG2	12	0.08
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG3	12	0.08
(1,1874)	1:B:53:THR:HB	1:B:54:THR:H	20	0.08
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	8	0.08
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	8	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	8	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	8	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	8	0.08
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	8	0.08
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	9	0.08
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	19	0.08
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD11	3	0.08
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD12	3	0.08
(1,1559)	1:B:31:LEU:HD21	1:B:67:LEU:HD13	3	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD11	3	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD12	3	0.08
(1,1559)	1:B:31:LEU:HD22	1:B:67:LEU:HD13	3	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD11	3	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD12	3	0.08
(1,1559)	1:B:31:LEU:HD23	1:B:67:LEU:HD13	3	0.08
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG21	11	0.08
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG22	11	0.08
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG23	11	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG21	11	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG22	11	0.08
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG23	11	0.08
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	10	0.08
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	10	0.08
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	10	0.08
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	10	0.08
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	10	0.08
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	10	0.08
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD11	19	0.08
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD12	19	0.08
(1,1442)	1:B:25:GLY:HA3	1:B:28:LEU:HD13	19	0.08
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	17	0.08
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	17	0.08
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	17	0.08
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	17	0.08
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD21	8	0.08
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD22	8	0.08
(1,1245)	1:A:101:LEU:HA	1:A:101:LEU:HD23	8	0.08
(1,1217)	1:A:96:VAL:HA	1:A:100:HIS:HD2	12	0.08
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG11	2	0.08
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG12	2	0.08
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG13	2	0.08
(1,994)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	2	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,994)	1:A:73:GLU:HG2	1:A:78:TYR:HD2	2	0.07
(1,994)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	2	0.07
(1,994)	1:A:73:GLU:HG3	1:A:78:TYR:HD2	2	0.07
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	16	0.07
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG3	16	0.07
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	16	0.07
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG3	16	0.07
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	13	0.07
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	13	0.07
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	13	0.07
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	13	0.07
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	13	0.07
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	13	0.07
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	13	0.07
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	13	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	14	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	14	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	14	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	15	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	15	0.07
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	15	0.07
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	7	0.07
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	7	0.07
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD21	15	0.07
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD22	15	0.07
(1,833)	1:A:62:LEU:HA	1:A:67:LEU:HD23	15	0.07
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	5	0.07
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	5	0.07
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	5	0.07
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	13	0.07
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	13	0.07
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	13	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	17	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	17	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	17	0.07
(1,522)	1:A:38:GLU:HG2	1:A:39:ARG:H	5	0.07
(1,522)	1:A:38:GLU:HG3	1:A:39:ARG:H	5	0.07
(1,522)	1:A:38:GLU:HG2	1:A:39:ARG:H	8	0.07
(1,522)	1:A:38:GLU:HG3	1:A:39:ARG:H	8	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB1	3	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB2	3	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB3	3	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,474)	1:A:33:LEU:HG	1:A:39:ARG:HE	15	0.07
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	14	0.07
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	14	0.07
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	14	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	14	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	14	0.07
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	14	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	14	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	14	0.07
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	14	0.07
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD11	12	0.07
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD12	12	0.07
(1,407)	1:A:31:LEU:HA	1:A:62:LEU:HD13	12	0.07
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	11	0.07
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	11	0.07
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	11	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	11	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	11	0.07
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	11	0.07
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	5	0.07
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	5	0.07
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	5	0.07
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	16	0.07
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	16	0.07
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	7	0.07
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	4	0.07
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	19	0.07
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	19	0.07
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	19	0.07
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	19	0.07
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	19	0.07
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	19	0.07
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	19	0.07
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	19	0.07
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	19	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2351)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	15	0.07
(1,2351)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	15	0.07
(1,2351)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	15	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	5	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	5	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	5	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	5	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	11	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	11	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	11	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	11	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG11	3	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG12	3	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG13	3	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG11	8	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG12	8	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG13	8	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG11	18	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG12	18	0.07
(1,2312)	1:B:93:VAL:H	1:B:93:VAL:HG13	18	0.07
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	19	0.07
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	19	0.07
(1,2152)	1:B:76:ARG:H	1:B:76:ARG:HG2	2	0.07
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	8	0.07
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	8	0.07
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	15	0.07
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	15	0.07
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	15	0.07
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	17	0.07
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	17	0.07
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	17	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	7	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	7	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	5	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	5	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	5	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	4	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	4	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	4	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE1	15	0.07
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE2	15	0.07
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	15	0.07
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	15	0.07
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	15	0.07
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	15	0.07
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	15	0.07
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	15	0.07
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	19	0.07
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	19	0.07
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	19	0.07
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	19	0.07
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	19	0.07
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	19	0.07
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	19	0.07
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	19	0.07
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	19	0.07
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	6	0.07
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	6	0.07
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	6	0.07
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	6	0.07
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD2	4	0.07
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD3	4	0.07
(1,1254)	1:A:102:GLU:H	1:A:102:GLU:HG2	4	0.07
(1,1254)	1:A:102:GLU:H	1:A:102:GLU:HG3	4	0.07
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	14	0.07
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	14	0.07
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	14	0.07
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	16	0.07
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	16	0.07
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	16	0.07
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	16	0.07
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG11	10	0.07
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG12	10	0.07
(1,1183)	1:A:93:VAL:H	1:A:93:VAL:HG13	10	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	16	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	16	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	16	0.07
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	15	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	15	0.07
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	15	0.06
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	15	0.06
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	15	0.06
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	15	0.06
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	9	0.06
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	9	0.06
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	9	0.06
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	9	0.06
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	9	0.06
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	9	0.06
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	9	0.06
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	9	0.06
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	8	0.06
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	8	0.06
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	8	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD11	8	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD12	8	0.06
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD13	8	0.06
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	1	0.06
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	1	0.06
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	1	0.06
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	16	0.06
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	16	0.06
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	16	0.06
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	4	0.06
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	4	0.06
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	4	0.06
(1,879)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	14	0.06
(1,879)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	14	0.06
(1,879)	1:A:65:GLY:HA3	1:A:67:LEU:HB2	14	0.06
(1,879)	1:A:65:GLY:HA3	1:A:67:LEU:HB3	14	0.06
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	2	0.06
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	2	0.06
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	2	0.06
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	2	0.06
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	20	0.06
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	20	0.06
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	20	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG2	7	0.06
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG3	7	0.06
(1,708)	1:A:50:MET:HE1	1:A:55:ALA:H	9	0.06
(1,708)	1:A:50:MET:HE2	1:A:55:ALA:H	9	0.06
(1,708)	1:A:50:MET:HE3	1:A:55:ALA:H	9	0.06
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	19	0.06
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	19	0.06
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	19	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	19	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	19	0.06
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	19	0.06
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	10	0.06
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	10	0.06
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	10	0.06
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	10	0.06
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	10	0.06
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	10	0.06
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	15	0.06
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	15	0.06
(1,430)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	15	0.06
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	15	0.06
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	15	0.06
(1,430)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	15	0.06
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	15	0.06
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	15	0.06
(1,430)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	15	0.06
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	9	0.06
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	9	0.06
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	9	0.06
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	9	0.06
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	9	0.06
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	9	0.06
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE1	20	0.06
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE2	20	0.06
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE3	20	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE1	20	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE2	20	0.06
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE3	20	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	8	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	8	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	8	0.06
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	8	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	8	0.06
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	8	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	17	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	17	0.06
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	17	0.06
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	17	0.06
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	17	0.06
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	17	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	13	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	13	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	13	0.06
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	10	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	18	0.06
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	20	0.06
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	20	0.06
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	20	0.06
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	18	0.06
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	9	0.06
(1,2568)	1:B:66:GLY:N	1:B:63:LYS:O	3	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	19	0.06
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	4	0.06
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	9	0.06
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	13	0.06
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	4	0.06
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	5	0.06
(1,2454)	1:A:66:GLY:N	1:A:63:LYS:O	15	0.06
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	2	0.06
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	6	0.06
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	6	0.06
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	6	0.06
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	6	0.06
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	6	0.06
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	6	0.06
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	6	0.06
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	6	0.06
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	6	0.06
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	1	0.06
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	1	0.06
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	1	0.06
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	1	0.06
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	11	0.06
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	11	0.06
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	11	0.06
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	11	0.06
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG11	8	0.06
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG12	8	0.06
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG13	8	0.06
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	19	0.06
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	19	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	4	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	4	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	4	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	4	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	4	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	4	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	4	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	4	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	9	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	9	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	9	0.06
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	9	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	9	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	9	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	9	0.06
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	9	0.06
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	6	0.06
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	6	0.06
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	6	0.06
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	17	0.06
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	17	0.06
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	17	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	17	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	17	0.06
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	17	0.06
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	14	0.06
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	14	0.06
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	4	0.06
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	4	0.06
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	4	0.06
(1,1876)	1:B:53:THR:HG21	1:B:54:THR:H	9	0.06
(1,1876)	1:B:53:THR:HG22	1:B:54:THR:H	9	0.06
(1,1876)	1:B:53:THR:HG23	1:B:54:THR:H	9	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	5	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	5	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	5	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	5	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	5	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	5	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	16	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	16	0.06
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	16	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	16	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	16	0.06
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	16	0.06
(1,1818)	1:B:48:THR:HB	1:B:50:MET:HG2	19	0.06
(1,1818)	1:B:48:THR:HB	1:B:50:MET:HG3	19	0.06
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	10	0.06
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	10	0.06
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	8	0.06
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	8	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	8	0.06
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	8	0.06
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	8	0.06
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	8	0.06
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG11	2	0.06
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG12	2	0.06
(1,1566)	1:B:31:LEU:HD21	1:B:86:VAL:HG13	2	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG11	2	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG12	2	0.06
(1,1566)	1:B:31:LEU:HD22	1:B:86:VAL:HG13	2	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG11	2	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG12	2	0.06
(1,1566)	1:B:31:LEU:HD23	1:B:86:VAL:HG13	2	0.06
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	9	0.06
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	9	0.06
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	9	0.06
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	9	0.06
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	9	0.06
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	9	0.06
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	1	0.06
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	1	0.06
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	1	0.06
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	1	0.06
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	1	0.06
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	1	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	1	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	1	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	1	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	8	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	8	0.06
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	8	0.06
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	11	0.06
(1,1441)	1:B:25:GLY:HA2	1:B:28:LEU:HB3	11	0.06
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB2	11	0.06
(1,1441)	1:B:25:GLY:HA3	1:B:28:LEU:HB3	11	0.06
(1,1374)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	5	0.06
(1,1374)	1:B:18:VAL:HG11	1:B:65:GLY:HA3	5	0.06
(1,1374)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	5	0.06
(1,1374)	1:B:18:VAL:HG12	1:B:65:GLY:HA3	5	0.06
(1,1374)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	5	0.06
(1,1374)	1:B:18:VAL:HG13	1:B:65:GLY:HA3	5	0.06
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA2	8	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA3	8	0.06
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	20	0.06
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	20	0.06
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD2	2	0.06
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD3	2	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	14	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	14	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	14	0.06
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	8	0.06
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	8	0.06
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	8	0.06
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	8	0.06
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	8	0.06
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	8	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD11	2	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD12	2	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD13	2	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD21	2	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD22	2	0.06
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD23	2	0.06
(1,1255)	1:A:107:HIS:HB2	1:A:108:HIS:H	4	0.06
(1,1255)	1:A:107:HIS:HB3	1:A:108:HIS:H	4	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG11	2	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG12	2	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG13	2	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG11	10	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG12	10	0.06
(1,1150)	1:A:90:PHE:HA	1:A:93:VAL:HG13	10	0.06
(1,1057)	1:A:81:ILE:HG12	1:A:87:ALA:HA	3	0.06
(1,1057)	1:A:81:ILE:HG13	1:A:87:ALA:HA	3	0.06
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	1	0.06
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	1	0.06
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	19	0.06
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	19	0.06
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD12	6	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD13	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD12	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD13	6	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD12	6	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD13	6	0.05
(1,974)	1:A:72:ARG:HA	1:A:72:ARG:HD2	6	0.05
(1,974)	1:A:72:ARG:HA	1:A:72:ARG:HD3	6	0.05
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	10	0.05
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	10	0.05
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	10	0.05
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	10	0.05
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	10	0.05
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	10	0.05
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	10	0.05
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	10	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB1	7	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB2	7	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB3	7	0.05
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	5	0.05
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	5	0.05
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	5	0.05
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	10	0.05
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	10	0.05
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	10	0.05
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	19	0.05
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	19	0.05
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	19	0.05
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	20	0.05
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	20	0.05
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	20	0.05
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG11	10	0.05
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG12	10	0.05
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG13	10	0.05
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD11	11	0.05
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD12	11	0.05
(1,886)	1:A:67:LEU:HA	1:A:67:LEU:HD13	11	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	19	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	19	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	19	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	19	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	19	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	19	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	20	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	20	0.05
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	20	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	20	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	20	0.05
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	20	0.05
(1,870)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	17	0.05
(1,870)	1:A:63:LYS:HG2	1:A:79:TYR:HE2	17	0.05
(1,870)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	17	0.05
(1,870)	1:A:63:LYS:HG3	1:A:79:TYR:HE2	17	0.05
(1,863)	1:A:63:LYS:HE2	1:A:70:ALA:H	11	0.05
(1,863)	1:A:63:LYS:HE3	1:A:70:ALA:H	11	0.05
(1,861)	1:A:63:LYS:HE2	1:A:69:GLU:HA	11	0.05
(1,861)	1:A:63:LYS:HE3	1:A:69:GLU:HA	11	0.05
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	20	0.05
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	20	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	12	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	12	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	12	0.05
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	12	0.05
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	12	0.05
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	12	0.05
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	20	0.05
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	20	0.05
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	20	0.05
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	4	0.05
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	4	0.05
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	4	0.05
(1,541)	1:A:40:ALA:HA	1:A:78:TYR:HA	10	0.05
(1,474)	1:A:33:LEU:HG	1:A:39:ARG:HE	8	0.05
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	8	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	8	0.05
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	8	0.05
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	8	0.05
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	8	0.05
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	8	0.05
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HG	4	0.05
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HG	4	0.05
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HG	4	0.05
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	17	0.05
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA3	17	0.05
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	17	0.05
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA3	17	0.05
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	17	0.05
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA3	17	0.05
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	8	0.05
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	8	0.05
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	8	0.05
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	8	0.05
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	8	0.05
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	8	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE1	12	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE2	12	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE3	12	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE1	12	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE2	12	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE3	12	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE1	19	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE2	19	0.05
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE3	19	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE1	19	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE2	19	0.05
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE3	19	0.05
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	6	0.05
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	6	0.05
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	6	0.05
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	11	0.05
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	11	0.05
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	11	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD21	11	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD22	11	0.05
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD23	11	0.05
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	20	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	20	0.05
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	20	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	12	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	14	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	14	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	14	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	18	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	18	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	18	0.05
(1,278)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	14	0.05
(1,278)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	14	0.05
(1,278)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	14	0.05
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	8	0.05
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	13	0.05
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	18	0.05
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	13	0.05
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	7	0.05
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	1	0.05
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	2	0.05
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	5	0.05
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	11	0.05
(1,2454)	1:A:66:GLY:N	1:A:63:LYS:O	14	0.05
(1,2403)	1:A:22:LEU:H	1:A:18:VAL:O	6	0.05
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	5	0.05
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	13	0.05
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	17	0.05
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	19	0.05
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	5	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	5	0.05
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	5	0.05
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	5	0.05
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	5	0.05
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	5	0.05
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	5	0.05
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	5	0.05
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	5	0.05
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD21	2	0.05
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD22	2	0.05
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD23	2	0.05
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	3	0.05
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	3	0.05
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	3	0.05
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	3	0.05
(1,2345)	1:B:96:VAL:HA	1:B:99:GLU:HB2	18	0.05
(1,2345)	1:B:96:VAL:HA	1:B:99:GLU:HB3	18	0.05
(1,2290)	1:B:91:ALA:HA	1:B:94:GLN:HE21	15	0.05
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	3	0.05
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA3	3	0.05
(1,2270)	1:B:89:LEU:HD21	1:B:93:VAL:HB	7	0.05
(1,2270)	1:B:89:LEU:HD22	1:B:93:VAL:HB	7	0.05
(1,2270)	1:B:89:LEU:HD23	1:B:93:VAL:HB	7	0.05
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	8	0.05
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE2	8	0.05
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE1	8	0.05
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE2	8	0.05
(1,2148)	1:B:76:ARG:HG2	1:B:77:GLN:H	3	0.05
(1,2148)	1:B:76:ARG:HG3	1:B:77:GLN:H	3	0.05
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	2	0.05
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE2	2	0.05
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	2	0.05
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE2	2	0.05
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	1	0.05
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	1	0.05
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	5	0.05
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	5	0.05
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	8	0.05
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	8	0.05
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	17	0.05
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	17	0.05
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	17	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	17	0.05
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	17	0.05
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	17	0.05
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	17	0.05
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	17	0.05
(1,2086)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	4	0.05
(1,2086)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	4	0.05
(1,2086)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	4	0.05
(1,2072)	1:B:69:GLU:HG2	1:B:82:ALA:HA	20	0.05
(1,2070)	1:B:69:GLU:HG3	1:B:82:ALA:HA	3	0.05
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	2	0.05
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	2	0.05
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	2	0.05
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	7	0.05
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	7	0.05
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	7	0.05
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	19	0.05
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	19	0.05
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	19	0.05
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	19	0.05
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	19	0.05
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	19	0.05
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	18	0.05
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	18	0.05
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	18	0.05
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	7	0.05
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	7	0.05
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	7	0.05
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	7	0.05
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	7	0.05
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	7	0.05
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	5	0.05
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	5	0.05
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	5	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	5	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	5	0.05
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	5	0.05
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	5	0.05
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	5	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	5	0.05
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	13	0.05
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	13	0.05
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	14	0.05
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	14	0.05
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	14	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB1	14	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB2	14	0.05
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB3	14	0.05
(1,1649)	1:B:38:GLU:HB2	1:B:80:ARG:HE	15	0.05
(1,1649)	1:B:38:GLU:HB3	1:B:80:ARG:HE	15	0.05
(1,1602)	1:B:33:LEU:HG	1:B:36:GLN:HE21	10	0.05
(1,1602)	1:B:33:LEU:HG	1:B:36:GLN:HE22	10	0.05
(1,1592)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD11	1:B:36:GLN:HG3	18	0.05
(1,1592)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD12	1:B:36:GLN:HG3	18	0.05
(1,1592)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD13	1:B:36:GLN:HG3	18	0.05
(1,1592)	1:B:33:LEU:HD21	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD21	1:B:36:GLN:HG3	18	0.05
(1,1592)	1:B:33:LEU:HD22	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD22	1:B:36:GLN:HG3	18	0.05
(1,1592)	1:B:33:LEU:HD23	1:B:36:GLN:HG2	18	0.05
(1,1592)	1:B:33:LEU:HD23	1:B:36:GLN:HG3	18	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	13	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	13	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	13	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	13	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	13	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	13	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	13	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	13	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	13	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	19	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	19	0.05
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	19	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	19	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	19	0.05
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	19	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	19	0.05
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	19	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	19	0.05
(1,1557)	1:B:31:LEU:HD21	1:B:67:LEU:HA	6	0.05
(1,1557)	1:B:31:LEU:HD22	1:B:67:LEU:HA	6	0.05
(1,1557)	1:B:31:LEU:HD23	1:B:67:LEU:HA	6	0.05
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG21	18	0.05
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG22	18	0.05
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG23	18	0.05
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG21	18	0.05
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG22	18	0.05
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG23	18	0.05
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	18	0.05
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	18	0.05
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	18	0.05
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	18	0.05
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	18	0.05
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	18	0.05
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	14	0.05
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	14	0.05
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	14	0.05
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	19	0.05
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	19	0.05
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	19	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD21	19	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD22	19	0.05
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD23	19	0.05
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	11	0.05
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	11	0.05
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	11	0.05
(1,1424)	1:B:22:LEU:HD11	1:B:93:VAL:HB	11	0.05
(1,1424)	1:B:22:LEU:HD12	1:B:93:VAL:HB	11	0.05
(1,1424)	1:B:22:LEU:HD13	1:B:93:VAL:HB	11	0.05
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	6	0.05
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	6	0.05
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	6	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	6	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	6	0.05
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	6	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	6	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	6	0.05
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	6	0.05
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD21	9	0.05
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD22	9	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD23	9	0.05
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	12	0.05
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	12	0.05
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	12	0.05
(1,1406)	1:B:21:ALA:HB1	1:B:65:GLY:HA3	10	0.05
(1,1406)	1:B:21:ALA:HB2	1:B:65:GLY:HA3	10	0.05
(1,1406)	1:B:21:ALA:HB3	1:B:65:GLY:HA3	10	0.05
(1,1399)	1:B:20:LYS:H	1:B:20:LYS:HD2	12	0.05
(1,1399)	1:B:20:LYS:H	1:B:20:LYS:HD3	12	0.05
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA2	14	0.05
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA3	14	0.05
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	6	0.05
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	6	0.05
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD2	8	0.05
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD3	8	0.05
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	17	0.05
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	17	0.05
(1,1280)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	17	0.05
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	17	0.05
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	17	0.05
(1,1280)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	17	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	4	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	4	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	4	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	4	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	4	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	4	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	4	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	4	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	4	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	18	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	18	0.05
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	18	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	18	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	18	0.05
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	18	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	18	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	18	0.05
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	18	0.05
(1,1180)	1:A:93:VAL:HG11	1:A:94:GLN:H	15	0.05
(1,1180)	1:A:93:VAL:HG12	1:A:94:GLN:H	15	0.05
(1,1180)	1:A:93:VAL:HG13	1:A:94:GLN:H	15	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	11	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	11	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	11	0.05
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	14	0.05
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	14	0.05
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	14	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	14	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	14	0.05
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	14	0.05
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	6	0.05
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	6	0.05
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	6	0.05
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	6	0.05
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	3	0.05
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	3	0.05
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	3	0.05
(1,1019)	1:A:76:ARG:HG2	1:A:77:GLN:H	2	0.05
(1,1019)	1:A:76:ARG:HG3	1:A:77:GLN:H	2	0.05
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	3	0.05
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	3	0.05
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	18	0.04
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	18	0.04
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	18	0.04
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	18	0.04
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	3	0.04
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	3	0.04
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	3	0.04
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	17	0.04
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	17	0.04
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	17	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	1	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	1	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	1	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	1	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	1	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	1	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	17	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	17	0.04
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	17	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	17	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	17	0.04
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	17	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,822)	1:A:60:GLN:HG2	1:A:61:ALA:HA	2	0.04
(1,822)	1:A:60:GLN:HG3	1:A:61:ALA:HA	2	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	19	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	19	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	19	0.04
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	6	0.04
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	6	0.04
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	6	0.04
(1,745)	1:A:53:THR:HB	1:A:54:THR:H	17	0.04
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	10	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	10	0.04
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	10	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD21	1:A:55:ALA:HB3	10	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD22	1:A:55:ALA:HB3	10	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB1	10	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB2	10	0.04
(1,738)	1:A:52:LEU:HD23	1:A:55:ALA:HB3	10	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	10	0.04
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	10	0.04
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	10	0.04
(1,67)	1:B:11:LEU:HD21	1:A:98:ASP:H	10	0.04
(1,67)	1:B:11:LEU:HD22	1:A:98:ASP:H	10	0.04
(1,67)	1:B:11:LEU:HD23	1:A:98:ASP:H	10	0.04
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	20	0.04
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	20	0.04
(1,615)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	20	0.04
(1,613)	1:A:42:GLU:HG2	1:A:52:LEU:HG	7	0.04
(1,613)	1:A:42:GLU:HG3	1:A:52:LEU:HG	7	0.04
(1,613)	1:A:42:GLU:HG2	1:A:52:LEU:HG	14	0.04
(1,613)	1:A:42:GLU:HG3	1:A:52:LEU:HG	14	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	2	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	2	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	2	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	2	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	2	0.04
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	2	0.04
(1,532)	1:A:39:ARG:HB2	1:A:39:ARG:HE	10	0.04
(1,532)	1:A:39:ARG:HB3	1:A:39:ARG:HE	10	0.04
(1,523)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	7	0.04
(1,523)	1:A:38:GLU:HG2	1:A:78:TYR:HB3	7	0.04
(1,523)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	7	0.04
(1,523)	1:A:38:GLU:HG3	1:A:78:TYR:HB3	7	0.04
(1,520)	1:A:38:GLU:HB2	1:A:80:ARG:HE	16	0.04
(1,520)	1:A:38:GLU:HB3	1:A:80:ARG:HE	16	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB1	4	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB2	4	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB3	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB1	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB2	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB3	4	0.04
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE21	12	0.04
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE22	12	0.04
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	15	0.04
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	15	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	15	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	15	0.04
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	15	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	15	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB1	15	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD21	1:A:43:ALA:HB3	15	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB1	15	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD22	1:A:43:ALA:HB3	15	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB1	15	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB2	15	0.04
(1,468)	1:A:33:LEU:HD23	1:A:43:ALA:HB3	15	0.04
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	10	0.04
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	10	0.04
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	10	0.04
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	10	0.04
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	10	0.04
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	10	0.04
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	10	0.04
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	18	0.04
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	18	0.04
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	18	0.04
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	18	0.04
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	18	0.04
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	18	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	14	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	14	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	14	0.04
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	14	0.04
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	14	0.04
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	14	0.04
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	11	0.04
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	11	0.04
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	11	0.04
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	4	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	4	0.04
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	4	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB1	4	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB2	4	0.04
(1,329)	1:A:27:ARG:HD3	1:A:61:ALA:HB3	4	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	3	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	3	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	3	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	14	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	14	0.04
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	14	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	12	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	12	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	12	0.04
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	17	0.04
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	11	0.04
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	11	0.04
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	11	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	20	0.04
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	15	0.04
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	15	0.04
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	15	0.04
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD11	15	0.04
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD12	15	0.04
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD13	15	0.04
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	5	0.04
(1,2587)	1:B:87:ALA:H	1:B:83:GLY:O	17	0.04
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	20	0.04
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	1	0.04
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	10	0.04
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	2	0.04
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	7	0.04
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	10	0.04
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	1	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	11	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	3	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	4	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	6	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	11	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	15	0.04
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	18	0.04
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	8	0.04
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	8	0.04
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	16	0.04
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	4	0.04
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	2	0.04
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	3	0.04
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	7	0.04
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	5	0.04
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	7	0.04
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	12	0.04
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	18	0.04
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	17	0.04
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	2	0.04
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	6	0.04
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	7	0.04
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	10	0.04
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	12	0.04
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	12	0.04
(1,2360)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	12	0.04
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	12	0.04
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	12	0.04
(1,2360)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	12	0.04
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	12	0.04
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	12	0.04
(1,2360)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	12	0.04
(1,2351)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	13	0.04
(1,2351)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	13	0.04
(1,2351)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	13	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	2	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	2	0.04
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	2	0.04
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	2	0.04
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	12	0.04
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	12	0.04
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	12	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	12	0.04
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	13	0.04
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	13	0.04
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	13	0.04
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	13	0.04
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG11	3	0.04
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG12	3	0.04
(1,2279)	1:B:90:PHE:HA	1:B:93:VAL:HG13	3	0.04
(1,2270)	1:B:89:LEU:HD21	1:B:93:VAL:HB	1	0.04
(1,2270)	1:B:89:LEU:HD22	1:B:93:VAL:HB	1	0.04
(1,2270)	1:B:89:LEU:HD23	1:B:93:VAL:HB	1	0.04
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD21	3	0.04
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD22	3	0.04
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD23	3	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	1	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	1	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	4	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	4	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	15	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	15	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	19	0.04
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	19	0.04
(1,2191)	1:B:81:ILE:HG21	1:B:83:GLY:H	6	0.04
(1,2191)	1:B:81:ILE:HG22	1:B:83:GLY:H	6	0.04
(1,2191)	1:B:81:ILE:HG23	1:B:83:GLY:H	6	0.04
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	12	0.04
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	12	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	12	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	12	0.04
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	16	0.04
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	16	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	16	0.04
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	16	0.04
(1,2129)	1:B:74:GLY:HA2	1:B:75:THR:HB	8	0.04
(1,2129)	1:B:74:GLY:HA3	1:B:75:THR:HB	8	0.04
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	10	0.04
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	10	0.04
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	10	0.04
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	10	0.04
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	10	0.04
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	10	0.04
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	10	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	10	0.04
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	19	0.04
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	19	0.04
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	19	0.04
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG11	17	0.04
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG12	17	0.04
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG13	17	0.04
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	15	0.04
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	15	0.04
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	15	0.04
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	15	0.04
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	15	0.04
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	15	0.04
(1,2008)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	3	0.04
(1,2008)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	3	0.04
(1,2008)	1:B:65:GLY:HA3	1:B:67:LEU:HB2	3	0.04
(1,2008)	1:B:65:GLY:HA3	1:B:67:LEU:HB3	3	0.04
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	2	0.04
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	2	0.04
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	2	0.04
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	2	0.04
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	4	0.04
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	4	0.04
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	4	0.04
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	4	0.04
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	3	0.04
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE2	3	0.04
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	3	0.04
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE2	3	0.04
(1,1986)	1:B:63:LYS:HB2	1:B:69:GLU:HA	3	0.04
(1,1986)	1:B:63:LYS:HB3	1:B:69:GLU:HA	3	0.04
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD21	3	0.04
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD22	3	0.04
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD23	3	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	15	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	15	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	15	0.04
(1,1882)	1:B:54:THR:HG21	1:B:57:ALA:H	10	0.04
(1,1882)	1:B:54:THR:HG22	1:B:57:ALA:H	10	0.04
(1,1882)	1:B:54:THR:HG23	1:B:57:ALA:H	10	0.04
(1,1876)	1:B:53:THR:HG21	1:B:54:THR:H	11	0.04
(1,1876)	1:B:53:THR:HG22	1:B:54:THR:H	11	0.04
(1,1876)	1:B:53:THR:HG23	1:B:54:THR:H	11	0.04
(1,1876)	1:B:53:THR:HG21	1:B:54:THR:H	12	0.04
(1,1876)	1:B:53:THR:HG22	1:B:54:THR:H	12	0.04
(1,1876)	1:B:53:THR:HG23	1:B:54:THR:H	12	0.04
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB1	9	0.04
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB2	9	0.04
(1,1831)	1:B:50:MET:HB2	1:B:55:ALA:HB3	9	0.04
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB1	9	0.04
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB2	9	0.04
(1,1831)	1:B:50:MET:HB3	1:B:55:ALA:HB3	9	0.04
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	14	0.04
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	14	0.04
(1,1745)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	14	0.04
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	2	0.04
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	2	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD11	4	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD12	4	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD13	4	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD21	4	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD22	4	0.04
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD23	4	0.04
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	10	0.04
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	10	0.04
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	10	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	10	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	10	0.04
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	10	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	10	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	10	0.04
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	10	0.04
(1,1629)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	6	0.04
(1,1629)	1:B:35:ALA:HB1	1:B:36:GLN:HE22	6	0.04
(1,1629)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	6	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1629)	1:B:35:ALA:HB2	1:B:36:GLN:HE22	6	0.04
(1,1629)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	6	0.04
(1,1629)	1:B:35:ALA:HB3	1:B:36:GLN:HE22	6	0.04
(1,1617)	1:B:34:LEU:HD21	1:B:37:GLY:H	8	0.04
(1,1617)	1:B:34:LEU:HD22	1:B:37:GLY:H	8	0.04
(1,1617)	1:B:34:LEU:HD23	1:B:37:GLY:H	8	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	20	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	20	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	20	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	5	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	5	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	5	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	5	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	5	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	5	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	7	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	7	0.04
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	7	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	7	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	7	0.04
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	7	0.04
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	7	0.04
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	7	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	7	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	7	0.04
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	12	0.04
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	12	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	12	0.04
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	12	0.04
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	7	0.04
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	7	0.04
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	7	0.04
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	7	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	7	0.04
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	7	0.04
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	17	0.04
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	17	0.04
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	17	0.04
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	17	0.04
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	17	0.04
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	17	0.04
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	11	0.04
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	11	0.04
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	11	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	11	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	11	0.04
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	11	0.04
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	11	0.04
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	11	0.04
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	11	0.04
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	11	0.04
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	11	0.04
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	11	0.04
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	11	0.04
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	11	0.04
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	11	0.04
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	11	0.04
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	11	0.04
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	11	0.04
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	11	0.04
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	11	0.04
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	11	0.04
(1,1407)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	2	0.04
(1,1407)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	2	0.04
(1,1407)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	2	0.04
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	4	0.04
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	4	0.04
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	4	0.04
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	4	0.04
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE2	11	0.04
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE3	11	0.04
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	14	0.04
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	14	0.04
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	14	0.04
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	14	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	1	0.04
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	1	0.04
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB1	13	0.04
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB2	13	0.04
(1,1261)	1:B:6:ASP:HA	1:B:9:ALA:HB3	13	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	4	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	4	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	4	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	7	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	7	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	7	0.04
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	14	0.04
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	14	0.04
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	14	0.04
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	14	0.04
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	14	0.04
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	14	0.04
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	14	0.04
(1,1090)	1:A:84:GLU:HG2	1:A:86:VAL:H	6	0.04
(1,1090)	1:A:84:GLU:HG3	1:A:86:VAL:H	6	0.04
(1,1076)	1:A:82:ALA:HB1	1:A:86:VAL:HB	8	0.04
(1,1076)	1:A:82:ALA:HB2	1:A:86:VAL:HB	8	0.04
(1,1076)	1:A:82:ALA:HB3	1:A:86:VAL:HB	8	0.04
(1,1075)	1:A:82:ALA:HB1	1:A:83:GLY:H	17	0.04
(1,1075)	1:A:82:ALA:HB2	1:A:83:GLY:H	17	0.04
(1,1075)	1:A:82:ALA:HB3	1:A:83:GLY:H	17	0.04
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	18	0.04
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	18	0.04
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	18	0.04
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	1	0.03
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	1	0.03
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	1	0.03
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	1	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	7	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB3	7	0.03
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	5	0.03
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG3	5	0.03
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	5	0.03
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG3	5	0.03
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	6	0.03
(1,985)	1:A:72:ARG:HD2	1:A:77:GLN:HG3	6	0.03
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	6	0.03
(1,985)	1:A:72:ARG:HD3	1:A:77:GLN:HG3	6	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	18	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	18	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	18	0.03
(1,957)	1:A:70:ALA:HB1	1:A:77:GLN:HE22	17	0.03
(1,957)	1:A:70:ALA:HB2	1:A:77:GLN:HE22	17	0.03
(1,957)	1:A:70:ALA:HB3	1:A:77:GLN:HE22	17	0.03
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	18	0.03
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	18	0.03
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	18	0.03
(1,941)	1:A:69:GLU:HG3	1:A:82:ALA:HA	9	0.03
(1,941)	1:A:69:GLU:HG3	1:A:82:ALA:HA	16	0.03
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG11	13	0.03
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG12	13	0.03
(1,919)	1:A:68:VAL:HG11	1:A:86:VAL:HG13	13	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG11	13	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG12	13	0.03
(1,919)	1:A:68:VAL:HG12	1:A:86:VAL:HG13	13	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG11	13	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG12	13	0.03
(1,919)	1:A:68:VAL:HG13	1:A:86:VAL:HG13	13	0.03
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	17	0.03
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	17	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	17	0.03
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD11	17	0.03
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD12	17	0.03
(1,90)	1:B:14:GLN:HG3	1:A:101:LEU:HD13	17	0.03
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	19	0.03
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	19	0.03
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	19	0.03
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	10	0.03
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	10	0.03
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	10	0.03
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	10	0.03
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	10	0.03
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	10	0.03
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	3	0.03
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	3	0.03
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	3	0.03
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	3	0.03
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	9	0.03
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	9	0.03
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	9	0.03
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	9	0.03
(1,863)	1:A:63:LYS:HE2	1:A:70:ALA:H	3	0.03
(1,863)	1:A:63:LYS:HE3	1:A:70:ALA:H	3	0.03
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	15	0.03
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	15	0.03
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	15	0.03
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	15	0.03
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	15	0.03
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	15	0.03
(1,861)	1:A:63:LYS:HE2	1:A:69:GLU:HA	4	0.03
(1,861)	1:A:63:LYS:HE3	1:A:69:GLU:HA	4	0.03
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	4	0.03
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	4	0.03
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG21	7	0.03
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG22	7	0.03
(1,840)	1:A:62:LEU:HB3	1:A:68:VAL:HG23	7	0.03
(1,822)	1:A:60:GLN:HG2	1:A:61:ALA:HA	1	0.03
(1,822)	1:A:60:GLN:HG3	1:A:61:ALA:HA	1	0.03
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	1	0.03
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	1	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	1	0.03
(1,745)	1:A:53:THR:HB	1:A:54:THR:H	15	0.03
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB1	18	0.03
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB2	18	0.03
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB3	18	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB1	18	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB2	18	0.03
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB3	18	0.03
(1,708)	1:A:50:MET:HE1	1:A:55:ALA:H	10	0.03
(1,708)	1:A:50:MET:HE2	1:A:55:ALA:H	10	0.03
(1,708)	1:A:50:MET:HE3	1:A:55:ALA:H	10	0.03
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB1	19	0.03
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB2	19	0.03
(1,702)	1:A:50:MET:HB2	1:A:55:ALA:HB3	19	0.03
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB1	19	0.03
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB2	19	0.03
(1,702)	1:A:50:MET:HB3	1:A:55:ALA:HB3	19	0.03
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	16	0.03
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	16	0.03
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	16	0.03
(1,67)	1:B:11:LEU:HD21	1:A:98:ASP:H	16	0.03
(1,67)	1:B:11:LEU:HD22	1:A:98:ASP:H	16	0.03
(1,67)	1:B:11:LEU:HD23	1:A:98:ASP:H	16	0.03
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	6	0.03
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	6	0.03
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	6	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	6	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	6	0.03
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	6	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	6	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	6	0.03
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	6	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	3	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	3	0.03
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	3	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	6	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	6	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	6	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	6	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	6	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	6	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	8	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	8	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	8	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	8	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	8	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	8	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	17	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	17	0.03
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	17	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	17	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	17	0.03
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	17	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD11	9	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD12	9	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD13	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD11	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD12	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD13	9	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	18	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	18	0.03
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	18	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	18	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	18	0.03
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	18	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	18	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	18	0.03
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	18	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	10	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	10	0.03
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	10	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD21	10	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD22	10	0.03
(1,58)	1:A:88:ARG:HB3	1:B:92:LEU:HD23	10	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	11	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	11	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	11	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD11	11	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD12	11	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD13	11	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	17	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	17	0.03
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	17	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD11	17	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD12	17	0.03
(1,57)	1:A:88:ARG:HB3	1:B:92:LEU:HD13	17	0.03
(1,541)	1:A:40:ALA:HA	1:A:78:TYR:HA	18	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	16	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	16	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	16	0.03
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG2	18	0.03
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG3	18	0.03
(1,504)	1:A:35:ALA:HB1	1:A:90:PHE:HD1	20	0.03
(1,504)	1:A:35:ALA:HB1	1:A:90:PHE:HD2	20	0.03
(1,504)	1:A:35:ALA:HB2	1:A:90:PHE:HD1	20	0.03
(1,504)	1:A:35:ALA:HB2	1:A:90:PHE:HD2	20	0.03
(1,504)	1:A:35:ALA:HB3	1:A:90:PHE:HD1	20	0.03
(1,504)	1:A:35:ALA:HB3	1:A:90:PHE:HD2	20	0.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	3	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	3	0.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	5	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	5	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	5	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	5	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	5	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	5	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	5	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	19	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	19	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	19	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	19	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	19	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	19	0.03
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	19	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	18	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE2	18	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	18	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE2	18	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	18	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE2	18	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	2	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	2	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	2	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	2	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	2	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	2	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	4	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	4	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	4	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	4	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	4	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	4	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	9	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	9	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	9	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	9	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	9	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	9	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	14	0.03
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	14	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	14	0.03
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	14	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	14	0.03
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	14	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,428)	1:A:31:LEU:HD21	1:A:67:LEU:HA	11	0.03
(1,428)	1:A:31:LEU:HD22	1:A:67:LEU:HA	11	0.03
(1,428)	1:A:31:LEU:HD23	1:A:67:LEU:HA	11	0.03
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	14	0.03
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	14	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	14	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	14	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	14	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	14	0.03
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	15	0.03
(1,419)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	15	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	15	0.03
(1,419)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	15	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	15	0.03
(1,419)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	15	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	3	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	3	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	3	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	3	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	3	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	3	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	18	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	18	0.03
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	18	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	18	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	18	0.03
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	18	0.03
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	20	0.03
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	20	0.03
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	20	0.03
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	20	0.03
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	20	0.03
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	20	0.03
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	13	0.03
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	13	0.03
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	13	0.03
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	13	0.03
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	7	0.03
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	7	0.03
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	7	0.03
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	7	0.03
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	7	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	7	0.03
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	15	0.03
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	15	0.03
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	15	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	15	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	15	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	15	0.03
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	18	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	13	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	12	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	12	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	12	0.03
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	13	0.03
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	13	0.03
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	13	0.03
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	10	0.03
(1,2583)	1:B:80:ARG:H	1:B:69:GLU:O	9	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE2	8	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE3	8	0.03
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	12	0.03
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	18	0.03
(1,2569)	1:B:67:LEU:H	1:B:62:LEU:O	6	0.03
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	7	0.03
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	15	0.03
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	7	0.03
(1,2551)	1:B:58:ASN:H	1:B:54:THR:O	11	0.03
(1,2549)	1:B:57:ALA:H	1:B:53:THR:O	7	0.03
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	4	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	6	0.03
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	8	0.03
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	12	0.03
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	9	0.03
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	11	0.03
(1,2519)	1:B:32:ASP:H	1:B:28:LEU:O	8	0.03
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	10	0.03
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	16	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	2	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	3	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	6	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	9	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	14	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	16	0.03
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	18	0.03
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	3	0.03
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	5	0.03
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	7	0.03
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	8	0.03
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	10	0.03
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	11	0.03
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	12	0.03
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	15	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	1	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	7	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	9	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	12	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	14	0.03
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	20	0.03
(1,2493)	1:A:97:ALA:H	1:A:93:VAL:O	3	0.03
(1,2493)	1:A:97:ALA:H	1:A:93:VAL:O	11	0.03
(1,2489)	1:A:95:VAL:H	1:A:91:ALA:O	16	0.03
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	7	0.03
(1,2469)	1:A:80:ARG:H	1:A:69:GLU:O	4	0.03
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	16	0.03
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	12	0.03
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	15	0.03
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	1	0.03
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	8	0.03
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	11	0.03
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	1	0.03
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	11	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	13	0.03
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	16	0.03
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	17	0.03
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	15	0.03
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	9	0.03
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	20	0.03
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	16	0.03
(1,2403)	1:A:22:LEU:H	1:A:18:VAL:O	3	0.03
(1,2403)	1:A:22:LEU:H	1:A:18:VAL:O	16	0.03
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	4	0.03
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	15	0.03
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	8	0.03
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	14	0.03
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	15	0.03
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	16	0.03
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	3	0.03
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	15	0.03
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	16	0.03
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	18	0.03
(1,2378)	1:B:101:LEU:HD21	1:B:102:GLU:H	5	0.03
(1,2378)	1:B:101:LEU:HD22	1:B:102:GLU:H	5	0.03
(1,2378)	1:B:101:LEU:HD23	1:B:102:GLU:H	5	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD21	5	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD22	5	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD23	5	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD21	14	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD22	14	0.03
(1,2356)	1:B:97:ALA:HA	1:B:101:LEU:HD23	14	0.03
(1,2327)	1:B:95:VAL:HA	1:B:98:ASP:HB2	8	0.03
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	20	0.03
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	20	0.03
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	20	0.03
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	20	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD2	14	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD3	14	0.03
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD21	15	0.03
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD22	15	0.03
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD23	15	0.03
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG21	2	0.03
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG22	2	0.03
(1,2208)	1:B:82:ALA:H	1:B:86:VAL:HG23	2	0.03
(1,2191)	1:B:81:ILE:HG21	1:B:83:GLY:H	3	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2191)	1:B:81:ILE:HG22	1:B:83:GLY:H	3	0.03
(1,2191)	1:B:81:ILE:HG23	1:B:83:GLY:H	3	0.03
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG2	14	0.03
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG3	14	0.03
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG2	17	0.03
(1,2174)	1:B:80:ARG:H	1:B:80:ARG:HG3	17	0.03
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	20	0.03
(1,2147)	1:B:76:ARG:HD2	1:B:78:TYR:HE2	20	0.03
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	20	0.03
(1,2147)	1:B:76:ARG:HD3	1:B:78:TYR:HE2	20	0.03
(1,2123)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	8	0.03
(1,2123)	1:B:73:GLU:HG2	1:B:78:TYR:HD2	8	0.03
(1,2123)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	8	0.03
(1,2123)	1:B:73:GLU:HG3	1:B:78:TYR:HD2	8	0.03
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	16	0.03
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	16	0.03
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	16	0.03
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	16	0.03
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	16	0.03
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	16	0.03
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	16	0.03
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	16	0.03
(1,2096)	1:B:71:ARG:HB2	1:B:79:TYR:HA	2	0.03
(1,2096)	1:B:71:ARG:HB3	1:B:79:TYR:HA	2	0.03
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD21	6	0.03
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD22	6	0.03
(1,2030)	1:B:67:LEU:H	1:B:67:LEU:HD23	6	0.03
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG21	8	0.03
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG22	8	0.03
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG23	8	0.03
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	10	0.03
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	10	0.03
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	10	0.03
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	10	0.03
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	10	0.03
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	10	0.03
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	8	0.03
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	8	0.03
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	8	0.03
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	8	0.03
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	12	0.03
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	12	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	12	0.03
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	12	0.03
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	6	0.03
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE2	6	0.03
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	6	0.03
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE2	6	0.03
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	10	0.03
(1,1989)	1:B:63:LYS:HD2	1:B:79:TYR:HE2	10	0.03
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	10	0.03
(1,1989)	1:B:63:LYS:HD3	1:B:79:TYR:HE2	10	0.03
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD21	14	0.03
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD22	14	0.03
(1,1962)	1:B:62:LEU:HA	1:B:67:LEU:HD23	14	0.03
(1,1951)	1:B:60:GLN:HG2	1:B:61:ALA:HA	17	0.03
(1,1951)	1:B:60:GLN:HG3	1:B:61:ALA:HA	17	0.03
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG2	8	0.03
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG3	8	0.03
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	12	0.03
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	12	0.03
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	12	0.03
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	12	0.03
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	12	0.03
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	12	0.03
(1,1884)	1:B:54:THR:HG21	1:B:58:ASN:HD22	10	0.03
(1,1884)	1:B:54:THR:HG22	1:B:58:ASN:HD22	10	0.03
(1,1884)	1:B:54:THR:HG23	1:B:58:ASN:HD22	10	0.03
(1,1872)	1:B:52:LEU:H	1:B:52:LEU:HG	3	0.03
(1,1868)	1:B:52:LEU:HD11	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD11	1:B:56:SER:HB3	1	0.03
(1,1868)	1:B:52:LEU:HD12	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD12	1:B:56:SER:HB3	1	0.03
(1,1868)	1:B:52:LEU:HD13	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD13	1:B:56:SER:HB3	1	0.03
(1,1868)	1:B:52:LEU:HD21	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD21	1:B:56:SER:HB3	1	0.03
(1,1868)	1:B:52:LEU:HD22	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD22	1:B:56:SER:HB3	1	0.03
(1,1868)	1:B:52:LEU:HD23	1:B:56:SER:HB2	1	0.03
(1,1868)	1:B:52:LEU:HD23	1:B:56:SER:HB3	1	0.03
(1,1832)	1:B:50:MET:HB2	1:B:55:ALA:H	19	0.03
(1,1832)	1:B:50:MET:HB3	1:B:55:ALA:H	19	0.03
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	13	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	13	0.03
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	13	0.03
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	13	0.03
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	13	0.03
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	13	0.03
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	13	0.03
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	13	0.03
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	13	0.03
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	15	0.03
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	15	0.03
(1,1744)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	15	0.03
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	18	0.03
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	18	0.03
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	18	0.03
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	6	0.03
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	6	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD11	11	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD12	11	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD13	11	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD21	11	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD22	11	0.03
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD23	11	0.03
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	2	0.03
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	2	0.03
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	2	0.03
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	2	0.03
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	2	0.03
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	2	0.03
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	2	0.03
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	2	0.03
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	2	0.03
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE1	3	0.03
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE2	3	0.03
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	10	0.03
(1,1616)	1:B:34:LEU:HD11	1:B:80:ARG:HA	7	0.03
(1,1616)	1:B:34:LEU:HD12	1:B:80:ARG:HA	7	0.03
(1,1616)	1:B:34:LEU:HD13	1:B:80:ARG:HA	7	0.03
(1,1591)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	16	0.03
(1,1591)	1:B:33:LEU:HD11	1:B:36:GLN:HE22	16	0.03
(1,1591)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	16	0.03
(1,1591)	1:B:33:LEU:HD12	1:B:36:GLN:HE22	16	0.03
(1,1591)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	16	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1591)	1:B:33:LEU:HD13	1:B:36:GLN:HE22	16	0.03
(1,1591)	1:B:33:LEU:HD21	1:B:36:GLN:HE21	16	0.03
(1,1591)	1:B:33:LEU:HD21	1:B:36:GLN:HE22	16	0.03
(1,1591)	1:B:33:LEU:HD22	1:B:36:GLN:HE21	16	0.03
(1,1591)	1:B:33:LEU:HD22	1:B:36:GLN:HE22	16	0.03
(1,1591)	1:B:33:LEU:HD23	1:B:36:GLN:HE21	16	0.03
(1,1591)	1:B:33:LEU:HD23	1:B:36:GLN:HE22	16	0.03
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	1	0.03
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	1	0.03
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	1	0.03
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	1	0.03
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	1	0.03
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	1	0.03
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	3	0.03
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	3	0.03
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	3	0.03
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	3	0.03
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	3	0.03
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	3	0.03
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD11	4	0.03
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD12	4	0.03
(1,1533)	1:B:31:LEU:HA	1:B:34:LEU:HD13	4	0.03
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	11	0.03
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	11	0.03
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG21	16	0.03
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG22	16	0.03
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG23	16	0.03
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG21	16	0.03
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG22	16	0.03
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG23	16	0.03
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE1	1	0.03
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE2	1	0.03
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE3	1	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE1	1	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE2	1	0.03
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE3	1	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	8	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	8	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	8	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	8	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	8	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	8	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	14	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	14	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	14	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	14	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	14	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	14	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	16	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	16	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	16	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	16	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	16	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	16	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	18	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	18	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	18	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	18	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	18	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	18	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	19	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	19	0.03
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	19	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	19	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	19	0.03
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	19	0.03
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	5	0.03
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	5	0.03
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	5	0.03
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	5	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	8	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	8	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	11	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	11	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	17	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	17	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	15	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	15	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	15	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	20	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	20	0.03
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	20	0.03
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	17	0.03
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	17	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	17	0.03
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD21	17	0.03
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD22	17	0.03
(1,1444)	1:B:25:GLY:HA3	1:B:28:LEU:HD23	17	0.03
(1,1437)	1:B:23:ALA:H	1:B:24:ASN:H	14	0.03
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	1	0.03
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	1	0.03
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	1	0.03
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	2	0.03
(1,1392)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	2	0.03
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	2	0.03
(1,1392)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	2	0.03
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE2	6	0.03
(1,1387)	1:B:20:LYS:HA	1:B:20:LYS:HE3	6	0.03
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	1	0.03
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	1	0.03
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	1	0.03
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	1	0.03
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	10	0.03
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	10	0.03
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	10	0.03
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	10	0.03
(1,1279)	1:B:8:LYS:HB2	1:B:9:ALA:H	1	0.03
(1,1279)	1:B:8:LYS:HB3	1:B:9:ALA:H	1	0.03
(1,1279)	1:B:8:LYS:HB2	1:B:9:ALA:H	17	0.03
(1,1279)	1:B:8:LYS:HB3	1:B:9:ALA:H	17	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD11	1	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD12	1	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD13	1	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD21	1	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD22	1	0.03
(1,1277)	1:B:8:LYS:HA	1:B:11:LEU:HD23	1	0.03
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	6	0.03
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	6	0.03
(1,1231)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	6	0.03
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	6	0.03
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	6	0.03
(1,1231)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	6	0.03
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	6	0.03
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	6	0.03
(1,1231)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	6	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	19	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	19	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	19	0.03
(1,1217)	1:A:96:VAL:HA	1:A:100:HIS:HD2	14	0.03
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	1	0.03
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	1	0.03
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	1	0.03
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	1	0.03
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	20	0.03
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	20	0.03
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	20	0.03
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	20	0.03
(1,1180)	1:A:93:VAL:HG11	1:A:94:GLN:H	1	0.03
(1,1180)	1:A:93:VAL:HG12	1:A:94:GLN:H	1	0.03
(1,1180)	1:A:93:VAL:HG13	1:A:94:GLN:H	1	0.03
(1,1163)	1:A:91:ALA:HA	1:A:94:GLN:HG2	2	0.03
(1,1163)	1:A:91:ALA:HA	1:A:94:GLN:HG3	2	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	5	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	5	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	5	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	5	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	5	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	5	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	18	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	18	0.03
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	18	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	18	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	18	0.03
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	18	0.03
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	2	0.03
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	2	0.03
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	2	0.03
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG11	2	0.03
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG12	2	0.03
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG13	2	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB1	4	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB2	4	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB3	4	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB1	4	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB2	4	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB3	4	0.03
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	7	0.03
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	7	0.03
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	7	0.03
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	17	0.03
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	17	0.03
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	17	0.03
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD2	19	0.03
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD3	19	0.03
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	11	0.03
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE22	11	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	11	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE22	11	0.03
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	12	0.03
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE22	12	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	12	0.03
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE22	12	0.03
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	6	0.03
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE2	6	0.03
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	6	0.03
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE2	6	0.03
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	10	0.03
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	10	0.03
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	20	0.03
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	20	0.03
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	13	0.03
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	13	0.03
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	13	0.03
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	1	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	1	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	1	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	1	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	1	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	1	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	1	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	1	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	12	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	12	0.02
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	12	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	12	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	12	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	12	0.02
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	12	0.02
(1,965)	1:A:71:ARG:HB2	1:A:71:ARG:HE	16	0.02
(1,965)	1:A:71:ARG:HB3	1:A:71:ARG:HE	16	0.02
(1,956)	1:A:70:ALA:HB1	1:A:77:GLN:HE21	16	0.02
(1,956)	1:A:70:ALA:HB2	1:A:77:GLN:HE21	16	0.02
(1,956)	1:A:70:ALA:HB3	1:A:77:GLN:HE21	16	0.02
(1,941)	1:A:69:GLU:HG3	1:A:82:ALA:HA	5	0.02
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD21	20	0.02
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD22	20	0.02
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD23	20	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD21	20	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD22	20	0.02
(1,91)	1:B:14:GLN:HG3	1:A:101:LEU:HD23	20	0.02
(1,897)	1:A:67:LEU:HD11	1:A:86:VAL:HA	12	0.02
(1,897)	1:A:67:LEU:HD12	1:A:86:VAL:HA	12	0.02
(1,897)	1:A:67:LEU:HD13	1:A:86:VAL:HA	12	0.02
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG21	9	0.02
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG22	9	0.02
(1,890)	1:A:67:LEU:HA	1:A:86:VAL:HG23	9	0.02
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	3	0.02
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	3	0.02
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	3	0.02
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	3	0.02
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	3	0.02
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	3	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD11	8	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD12	8	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD13	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD11	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD12	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD13	8	0.02
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	7	0.02
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	7	0.02
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	7	0.02
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	7	0.02
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	12	0.02
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	12	0.02
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	12	0.02
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	12	0.02
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	12	0.02
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	13	0.02
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	13	0.02
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	19	0.02
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG3	19	0.02
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	10	0.02
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE22	10	0.02
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	10	0.02
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE22	10	0.02
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	10	0.02
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE22	10	0.02
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	3	0.02
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	3	0.02
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	3	0.02
(1,740)	1:A:52:LEU:HD11	1:A:56:SER:H	10	0.02
(1,740)	1:A:52:LEU:HD12	1:A:56:SER:H	10	0.02
(1,740)	1:A:52:LEU:HD13	1:A:56:SER:H	10	0.02
(1,740)	1:A:52:LEU:HD21	1:A:56:SER:H	10	0.02
(1,740)	1:A:52:LEU:HD22	1:A:56:SER:H	10	0.02
(1,740)	1:A:52:LEU:HD23	1:A:56:SER:H	10	0.02
(1,714)	1:A:50:MET:H	1:A:50:MET:HE1	9	0.02
(1,714)	1:A:50:MET:H	1:A:50:MET:HE2	9	0.02
(1,714)	1:A:50:MET:H	1:A:50:MET:HE3	9	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB1	3	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB2	3	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB3	3	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB1	3	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB2	3	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB3	3	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB1	15	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB2	15	0.02
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB3	15	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB1	15	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB2	15	0.02
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB3	15	0.02
(1,66)	1:B:11:LEU:HD11	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD12	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD13	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD21	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD22	1:A:98:ASP:HB2	18	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,66)	1:B:11:LEU:HD23	1:A:98:ASP:HB2	18	0.02
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	17	0.02
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	17	0.02
(1,648)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	17	0.02
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	17	0.02
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	17	0.02
(1,648)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	17	0.02
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	17	0.02
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	17	0.02
(1,648)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	17	0.02
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD21	9	0.02
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD22	9	0.02
(1,643)	1:A:44:ILE:HD11	1:A:59:LEU:HD23	9	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD21	9	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD22	9	0.02
(1,643)	1:A:44:ILE:HD12	1:A:59:LEU:HD23	9	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD21	9	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD22	9	0.02
(1,643)	1:A:44:ILE:HD13	1:A:59:LEU:HD23	9	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	9	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	9	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	9	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	17	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	17	0.02
(1,616)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	17	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	1	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	1	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	1	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	5	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	5	0.02
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	5	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	8	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	8	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	8	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	8	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	8	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	8	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	8	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	13	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	13	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	13	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	13	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	13	0.02
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	13	0.02
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	13	0.02
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	9	0.02
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	9	0.02
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	9	0.02
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	9	0.02
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	9	0.02
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	9	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	4	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	12	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	20	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	20	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	20	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	20	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	20	0.02
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	20	0.02
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	20	0.02
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	20	0.02
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	20	0.02
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	20	0.02
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	20	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	20	0.02
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	20	0.02
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	20	0.02
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	20	0.02
(1,572)	1:A:41:VAL:HB	1:A:79:TYR:HE1	2	0.02
(1,572)	1:A:41:VAL:HB	1:A:79:TYR:HE2	2	0.02
(1,547)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	1	0.02
(1,547)	1:A:40:ALA:HB1	1:A:42:GLU:HG3	1	0.02
(1,547)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	1	0.02
(1,547)	1:A:40:ALA:HB2	1:A:42:GLU:HG3	1	0.02
(1,547)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	1	0.02
(1,547)	1:A:40:ALA:HB3	1:A:42:GLU:HG3	1	0.02
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG2	1	0.02
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG3	1	0.02
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG2	5	0.02
(1,526)	1:A:38:GLU:H	1:A:38:GLU:HG3	5	0.02
(1,511)	1:A:36:GLN:HG2	1:A:37:GLY:H	2	0.02
(1,511)	1:A:36:GLN:HG3	1:A:37:GLY:H	2	0.02
(1,474)	1:A:33:LEU:HG	1:A:39:ARG:HE	3	0.02
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE21	6	0.02
(1,473)	1:A:33:LEU:HG	1:A:36:GLN:HE22	6	0.02
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HG3	7	0.02
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HG3	7	0.02
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HG3	7	0.02
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD21	1:A:36:GLN:HG3	7	0.02
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD22	1:A:36:GLN:HG3	7	0.02
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG2	7	0.02
(1,463)	1:A:33:LEU:HD23	1:A:36:GLN:HG3	7	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	8	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE2	8	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	8	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE2	8	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	8	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE2	8	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	14	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HE2	14	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	14	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HE2	14	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	14	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HE2	14	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	11	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	11	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	11	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	11	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	11	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	11	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	15	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	15	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	15	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	15	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	15	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	15	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	20	0.02
(1,438)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	20	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	20	0.02
(1,438)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	20	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	20	0.02
(1,438)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	20	0.02
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG11	17	0.02
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG12	17	0.02
(1,437)	1:A:31:LEU:HD21	1:A:86:VAL:HG13	17	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG11	17	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG12	17	0.02
(1,437)	1:A:31:LEU:HD22	1:A:86:VAL:HG13	17	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG11	17	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG12	17	0.02
(1,437)	1:A:31:LEU:HD23	1:A:86:VAL:HG13	17	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD11	16	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD12	16	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HD13	16	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD11	16	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD12	16	0.02
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HD13	16	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD11	16	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD12	16	0.02
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HD13	16	0.02
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	4	0.02
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA3	4	0.02
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	4	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA3	4	0.02
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	4	0.02
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA3	4	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	5	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	8	0.02
(1,381)	1:A:30:ILE:HD11	1:A:59:LEU:HA	3	0.02
(1,381)	1:A:30:ILE:HD12	1:A:59:LEU:HA	3	0.02
(1,381)	1:A:30:ILE:HD13	1:A:59:LEU:HA	3	0.02
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	8	0.02
(1,360)	1:A:29:GLN:HG3	1:A:48:THR:HB	8	0.02
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	9	0.02
(1,360)	1:A:29:GLN:HG3	1:A:48:THR:HB	9	0.02
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE1	8	0.02
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE2	8	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE1	8	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE2	8	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE1	8	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE2	8	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	5	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	5	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	5	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	14	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	14	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	14	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	8	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	8	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	8	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	19	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	19	0.02
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	19	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	2	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	2	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	2	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD21	2	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD22	2	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD23	2	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	7	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	7	0.02
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	7	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD21	7	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD22	7	0.02
(1,315)	1:A:25:GLY:HA3	1:A:28:LEU:HD23	7	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	2	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	2	0.02
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	2	0.02
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	4	0.02
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB3	4	0.02
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB2	4	0.02
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB3	4	0.02
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	11	0.02
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB3	11	0.02
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB2	11	0.02
(1,312)	1:A:25:GLY:HA3	1:A:28:LEU:HB3	11	0.02
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	8	0.02
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	17	0.02
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	17	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	17	0.02
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	17	0.02
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	17	0.02
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	17	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG13	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG13	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG13	4	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD21	5	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD22	5	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD23	5	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD21	5	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD22	5	0.02
(1,28)	1:A:14:GLN:HG3	1:B:101:LEU:HD23	5	0.02
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	1	0.02
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	1	0.02
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	1	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD2	16	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD3	16	0.02
(1,2611)	1:B:99:GLU:H	1:B:95:VAL:O	4	0.02
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	16	0.02
(1,2601)	1:B:94:GLN:H	1:B:90:PHE:O	12	0.02
(1,2595)	1:B:91:ALA:H	1:B:87:ALA:O	12	0.02
(1,2595)	1:B:91:ALA:H	1:B:87:ALA:O	14	0.02
(1,2587)	1:B:87:ALA:H	1:B:83:GLY:O	15	0.02
(1,2583)	1:B:80:ARG:H	1:B:69:GLU:O	3	0.02
(1,2579)	1:B:78:TYR:H	1:B:71:ARG:O	9	0.02
(1,2579)	1:B:78:TYR:H	1:B:71:ARG:O	19	0.02
(1,2575)	1:B:73:GLU:H	1:B:76:ARG:O	11	0.02
(1,2575)	1:B:73:GLU:H	1:B:76:ARG:O	15	0.02
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	8	0.02
(1,2569)	1:B:67:LEU:H	1:B:62:LEU:O	3	0.02
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	8	0.02
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	14	0.02
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	18	0.02
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	6	0.02
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	13	0.02
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	17	0.02
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	20	0.02
(1,2555)	1:B:60:GLN:H	1:B:56:SER:O	12	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	3	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	5	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	7	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	9	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	16	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	17	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	19	0.02
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	20	0.02
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	11	0.02
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	16	0.02
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	1	0.02
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	2	0.02
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	9	0.02
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	15	0.02
(1,2519)	1:B:32:ASP:H	1:B:28:LEU:O	17	0.02
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	8	0.02
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	12	0.02
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	11	0.02
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	15	0.02
(1,2510)	1:B:18:VAL:N	1:B:14:GLN:O	4	0.02
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	11	0.02
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	12	0.02
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	4	0.02
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	18	0.02
(1,2505)	1:B:16:ALA:H	1:B:12:LEU:O	7	0.02
(1,2505)	1:B:16:ALA:H	1:B:12:LEU:O	14	0.02
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	19	0.02
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	8	0.02
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	10	0.02
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	16	0.02
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	17	0.02
(1,2499)	1:B:11:LEU:H	1:B:8:LYS:O	19	0.02
(1,2493)	1:A:97:ALA:H	1:A:93:VAL:O	13	0.02
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	4	0.02
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	5	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	5	0.02
(1,2473)	1:A:87:ALA:H	1:A:83:GLY:O	4	0.02
(1,2469)	1:A:80:ARG:H	1:A:69:GLU:O	2	0.02
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	2	0.02
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	7	0.02
(1,2459)	1:A:71:ARG:H	1:A:78:TYR:O	12	0.02
(1,2455)	1:A:67:LEU:H	1:A:62:LEU:O	14	0.02
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	10	0.02
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	12	0.02
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	4	0.02
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	5	0.02
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	11	0.02
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	17	0.02
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	1	0.02
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	11	0.02
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	15	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	4	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	5	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	9	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	10	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	12	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	14	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	15	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	18	0.02
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	19	0.02
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	3	0.02
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	11	0.02
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	18	0.02
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	20	0.02
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	1	0.02
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	6	0.02
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	2	0.02
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	8	0.02
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	11	0.02
(1,2405)	1:A:32:ASP:H	1:A:28:LEU:O	2	0.02
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	1	0.02
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	8	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	18	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	18	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	18	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	18	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	18	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	18	0.02
(1,2397)	1:A:19:GLY:H	1:A:15:VAL:O	16	0.02
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	9	0.02
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	3	0.02
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	6	0.02
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	8	0.02
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	1	0.02
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	5	0.02
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	9	0.02
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	11	0.02
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	20	0.02
(1,2383)	1:B:102:GLU:H	1:B:102:GLU:HG2	7	0.02
(1,2383)	1:B:102:GLU:H	1:B:102:GLU:HG3	7	0.02
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	6	0.02
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	6	0.02
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	6	0.02
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	6	0.02
(1,2292)	1:B:91:ALA:HA	1:B:94:GLN:HG2	9	0.02
(1,2292)	1:B:91:ALA:HA	1:B:94:GLN:HG3	9	0.02
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	4	0.02
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA3	4	0.02
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	5	0.02
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA3	5	0.02
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG11	7	0.02
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG12	7	0.02
(1,2285)	1:B:90:PHE:HD1	1:B:93:VAL:HG13	7	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG11	7	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG12	7	0.02
(1,2285)	1:B:90:PHE:HD2	1:B:93:VAL:HG13	7	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	3	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	3	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	3	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG11	3	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG12	3	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG13	3	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	8	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	8	0.02
(1,2281)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	8	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG11	8	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG12	8	0.02
(1,2281)	1:B:90:PHE:HB3	1:B:93:VAL:HG13	8	0.02
(1,2270)	1:B:89:LEU:HD21	1:B:93:VAL:HB	17	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2270)	1:B:89:LEU:HD22	1:B:93:VAL:HB	17	0.02
(1,2270)	1:B:89:LEU:HD23	1:B:93:VAL:HB	17	0.02
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	6	0.02
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	6	0.02
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	5	0.02
(1,2220)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	5	0.02
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	5	0.02
(1,2220)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	5	0.02
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	10	0.02
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	10	0.02
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB1	7	0.02
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB2	7	0.02
(1,2196)	1:B:81:ILE:HG21	1:B:87:ALA:HB3	7	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB1	7	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB2	7	0.02
(1,2196)	1:B:81:ILE:HG22	1:B:87:ALA:HB3	7	0.02
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB1	7	0.02
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB2	7	0.02
(1,2196)	1:B:81:ILE:HG23	1:B:87:ALA:HB3	7	0.02
(1,2179)	1:B:81:ILE:HD11	1:B:82:ALA:H	11	0.02
(1,2179)	1:B:81:ILE:HD12	1:B:82:ALA:H	11	0.02
(1,2179)	1:B:81:ILE:HD13	1:B:82:ALA:H	11	0.02
(1,2179)	1:B:81:ILE:HD11	1:B:82:ALA:H	15	0.02
(1,2179)	1:B:81:ILE:HD12	1:B:82:ALA:H	15	0.02
(1,2179)	1:B:81:ILE:HD13	1:B:82:ALA:H	15	0.02
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	7	0.02
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	7	0.02
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	7	0.02
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	7	0.02
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	13	0.02
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	13	0.02
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	13	0.02
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	13	0.02
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	6	0.02
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	6	0.02
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	16	0.02
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	16	0.02
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	20	0.02
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	20	0.02
(1,2129)	1:B:74:GLY:HA2	1:B:75:THR:HB	2	0.02
(1,2129)	1:B:74:GLY:HA3	1:B:75:THR:HB	2	0.02
(1,2129)	1:B:74:GLY:HA2	1:B:75:THR:HB	3	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2129)	1:B:74:GLY:HA3	1:B:75:THR:HB	3	0.02
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	1	0.02
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE2	1	0.02
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE1	1	0.02
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE2	1	0.02
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	3	0.02
(1,2122)	1:B:73:GLU:HB2	1:B:78:TYR:HE2	3	0.02
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE1	3	0.02
(1,2122)	1:B:73:GLU:HB3	1:B:78:TYR:HE2	3	0.02
(1,210)	1:A:15:VAL:HA	1:A:18:VAL:HB	10	0.02
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	14	0.02
(1,2099)	1:B:71:ARG:HG2	1:B:78:TYR:HB3	14	0.02
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB2	14	0.02
(1,2099)	1:B:71:ARG:HG3	1:B:78:TYR:HB3	14	0.02
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH11	7	0.02
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH12	7	0.02
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH21	7	0.02
(1,2097)	1:B:71:ARG:HD2	1:B:71:ARG:HH22	7	0.02
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH11	7	0.02
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH12	7	0.02
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH21	7	0.02
(1,2097)	1:B:71:ARG:HD3	1:B:71:ARG:HH22	7	0.02
(1,2086)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	11	0.02
(1,2086)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	11	0.02
(1,2086)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	11	0.02
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB1	10	0.02
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB2	10	0.02
(1,2073)	1:B:69:GLU:HG2	1:B:82:ALA:HB3	10	0.02
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	9	0.02
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	9	0.02
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	6	0.02
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	6	0.02
(1,2024)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	6	0.02
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	6	0.02
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	6	0.02
(1,2024)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	6	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG21	3	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG22	3	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG23	3	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG21	16	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG22	16	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG23	16	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG21	19	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG22	19	0.02
(1,2019)	1:B:67:LEU:HA	1:B:86:VAL:HG23	19	0.02
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	2	0.02
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	2	0.02
(1,2012)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	2	0.02
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD21	2	0.02
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD22	2	0.02
(1,2012)	1:B:66:GLY:HA3	1:B:67:LEU:HD23	2	0.02
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	1	0.02
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	1	0.02
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	1	0.02
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	1	0.02
(1,1992)	1:B:63:LYS:HE2	1:B:70:ALA:H	8	0.02
(1,1992)	1:B:63:LYS:HE3	1:B:70:ALA:H	8	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	2	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	2	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	2	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	2	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	2	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	2	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	15	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	15	0.02
(1,1991)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	15	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	15	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	15	0.02
(1,1991)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	15	0.02
(1,1986)	1:B:63:LYS:HB2	1:B:69:GLU:HA	20	0.02
(1,1986)	1:B:63:LYS:HB3	1:B:69:GLU:HA	20	0.02
(1,1951)	1:B:60:GLN:HG2	1:B:61:ALA:HA	7	0.02
(1,1951)	1:B:60:GLN:HG3	1:B:61:ALA:HA	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	2	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	2	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	2	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	19	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	19	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	19	0.02
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB1	4	0.02
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB2	4	0.02
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB3	4	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB1	4	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB2	4	0.02
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB3	4	0.02
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE1	14	0.02
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE2	14	0.02
(1,1816)	1:B:48:THR:HA	1:B:50:MET:HE3	14	0.02
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	7	0.02
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	7	0.02
(1,1777)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	7	0.02
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	7	0.02
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	7	0.02
(1,1777)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	7	0.02
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	7	0.02
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	7	0.02
(1,1777)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	7	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	7	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	7	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	7	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	7	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	7	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	7	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	14	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	14	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	18	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	18	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	18	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	18	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	18	0.02
(1,1741)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	18	0.02
(1,1741)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	18	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	5	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	5	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	5	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB1	5	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB2	5	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB3	5	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	11	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	11	0.02
(1,1740)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	11	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB1	11	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB2	11	0.02
(1,1740)	1:B:42:GLU:HG3	1:B:45:ALA:HB3	11	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	7	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	7	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	7	0.02
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	7	0.02
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	7	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	7	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	7	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	7	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	7	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	18	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	18	0.02
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	18	0.02
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	18	0.02
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	18	0.02
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	18	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	18	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	18	0.02
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	18	0.02
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE1	8	0.02
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE2	8	0.02
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	6	0.02
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	20	0.02
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG2	2	0.02
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG3	2	0.02
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG2	13	0.02
(1,1655)	1:B:38:GLU:H	1:B:38:GLU:HG3	13	0.02
(1,1653)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	12	0.02
(1,1653)	1:B:38:GLU:HG2	1:B:78:TYR:HD2	12	0.02
(1,1653)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	12	0.02
(1,1653)	1:B:38:GLU:HG3	1:B:78:TYR:HD2	12	0.02
(1,1620)	1:B:34:LEU:HD21	1:B:80:ARG:HA	8	0.02
(1,1620)	1:B:34:LEU:HD22	1:B:80:ARG:HA	8	0.02
(1,1620)	1:B:34:LEU:HD23	1:B:80:ARG:HA	8	0.02
(1,1568)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	14	0.02
(1,1568)	1:B:31:LEU:HD21	1:B:90:PHE:HE2	14	0.02
(1,1568)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	14	0.02
(1,1568)	1:B:31:LEU:HD22	1:B:90:PHE:HE2	14	0.02
(1,1568)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	14	0.02
(1,1568)	1:B:31:LEU:HD23	1:B:90:PHE:HE2	14	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	5	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	5	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	5	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	5	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	5	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	5	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	6	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	6	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	6	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	6	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	6	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	6	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	9	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	9	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	9	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	9	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	9	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	9	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	11	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	11	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	11	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	11	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	11	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	11	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	16	0.02
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	16	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	16	0.02
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	16	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	16	0.02
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	16	0.02
(1,1548)	1:B:31:LEU:HD11	1:B:67:LEU:HB2	3	0.02
(1,1548)	1:B:31:LEU:HD11	1:B:67:LEU:HB3	3	0.02
(1,1548)	1:B:31:LEU:HD12	1:B:67:LEU:HB2	3	0.02
(1,1548)	1:B:31:LEU:HD12	1:B:67:LEU:HB3	3	0.02
(1,1548)	1:B:31:LEU:HD13	1:B:67:LEU:HB2	3	0.02
(1,1548)	1:B:31:LEU:HD13	1:B:67:LEU:HB3	3	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD11	20	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD12	20	0.02
(1,1537)	1:B:31:LEU:HA	1:B:81:ILE:HD13	20	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	11	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	11	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	11	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	11	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	11	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	11	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	11	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	11	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	11	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	12	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	12	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	12	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	12	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	12	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	12	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	12	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	12	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	19	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	19	0.02
(1,1524)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	19	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	19	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	19	0.02
(1,1524)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	19	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	19	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	19	0.02
(1,1524)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	19	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	14	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	14	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	14	0.02
(1,1509)	1:B:30:ILE:HD11	1:B:58:ASN:H	18	0.02
(1,1509)	1:B:30:ILE:HD12	1:B:58:ASN:H	18	0.02
(1,1509)	1:B:30:ILE:HD13	1:B:58:ASN:H	18	0.02
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG21	12	0.02
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG22	12	0.02
(1,1490)	1:B:29:GLN:HG2	1:B:48:THR:HG23	12	0.02
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG21	12	0.02
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG22	12	0.02
(1,1490)	1:B:29:GLN:HG3	1:B:48:THR:HG23	12	0.02
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE1	4	0.02
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE2	4	0.02
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE3	4	0.02
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE1	4	0.02
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE2	4	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE3	4	0.02
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	13	0.02
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	13	0.02
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	13	0.02
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	13	0.02
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	13	0.02
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	13	0.02
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	9	0.02
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	9	0.02
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	9	0.02
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	9	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	3	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	3	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	3	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	3	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	3	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	3	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	4	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	4	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	4	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	4	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	4	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	4	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	11	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	11	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	11	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	11	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	11	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	11	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	20	0.02
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	20	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	20	0.02
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	20	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	20	0.02
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	20	0.02
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	4	0.02
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	4	0.02
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	12	0.02
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	12	0.02
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	12	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	8	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	8	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	8	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	17	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	17	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	17	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	18	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	18	0.02
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	18	0.02
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	19	0.02
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	19	0.02
(1,1428)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	19	0.02
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	19	0.02
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	19	0.02
(1,1428)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	19	0.02
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	19	0.02
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	19	0.02
(1,1428)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	19	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG11	4	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG12	4	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:93:VAL:HG13	4	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG11	4	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG12	4	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:93:VAL:HG13	4	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG11	4	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG12	4	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:93:VAL:HG13	4	0.02
(1,1424)	1:B:22:LEU:HD11	1:B:93:VAL:HB	15	0.02
(1,1424)	1:B:22:LEU:HD12	1:B:93:VAL:HB	15	0.02
(1,1424)	1:B:22:LEU:HD13	1:B:93:VAL:HB	15	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	17	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	17	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	17	0.02
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	17	0.02
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	17	0.02
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	17	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	17	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	17	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	17	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	20	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	20	0.02
(1,1422)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	20	0.02
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	20	0.02
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	20	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1422)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	20	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	20	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	20	0.02
(1,1422)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	20	0.02
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD21	1	0.02
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD22	1	0.02
(1,1415)	1:B:22:LEU:HA	1:B:28:LEU:HD23	1	0.02
(1,14)	1:A:12:LEU:HD21	1:B:28:LEU:H	19	0.02
(1,14)	1:A:12:LEU:HD22	1:B:28:LEU:H	19	0.02
(1,14)	1:A:12:LEU:HD23	1:B:28:LEU:H	19	0.02
(1,1359)	1:B:17:ARG:H	1:B:17:ARG:HD2	2	0.02
(1,1359)	1:B:17:ARG:H	1:B:17:ARG:HD3	2	0.02
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA2	16	0.02
(1,1358)	1:B:17:ARG:HA	1:B:65:GLY:HA3	16	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	2	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	2	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	10	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	10	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	15	0.02
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	15	0.02
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD2	11	0.02
(1,1330)	1:B:14:GLN:HA	1:B:17:ARG:HD3	11	0.02
(1,1279)	1:B:8:LYS:HB2	1:B:9:ALA:H	2	0.02
(1,1279)	1:B:8:LYS:HB3	1:B:9:ALA:H	2	0.02
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	11	0.02
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	11	0.02
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD2	14	0.02
(1,1275)	1:B:8:LYS:HA	1:B:8:LYS:HD3	14	0.02
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	7	0.02
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	7	0.02
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	7	0.02
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	11	0.02
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	11	0.02
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	11	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	2	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	2	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	2	0.02
(1,1216)	1:A:96:VAL:HA	1:A:99:GLU:HB2	12	0.02
(1,1216)	1:A:96:VAL:HA	1:A:99:GLU:HB3	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	5	0.02
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	5	0.02
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	5	0.02
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	5	0.02
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	8	0.02
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	8	0.02
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	8	0.02
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	8	0.02
(1,1161)	1:A:91:ALA:HA	1:A:94:GLN:HE21	17	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	12	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	12	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	12	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	12	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	12	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	12	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	13	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	13	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	13	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	13	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	13	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	13	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	15	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	15	0.02
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	15	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	15	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	15	0.02
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	15	0.02
(1,1141)	1:A:89:LEU:HD21	1:A:93:VAL:HB	12	0.02
(1,1141)	1:A:89:LEU:HD22	1:A:93:VAL:HB	12	0.02
(1,1141)	1:A:89:LEU:HD23	1:A:93:VAL:HB	12	0.02
(1,1141)	1:A:89:LEU:HD21	1:A:93:VAL:HB	20	0.02
(1,1141)	1:A:89:LEU:HD22	1:A:93:VAL:HB	20	0.02
(1,1141)	1:A:89:LEU:HD23	1:A:93:VAL:HB	20	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	1	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	1	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	1	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	3	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	3	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	3	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	6	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	6	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	6	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	8	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	8	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	8	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	12	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	12	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	12	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	17	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	17	0.02
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	17	0.02
(1,1120)	1:A:87:ALA:H	1:A:88:ARG:HG2	14	0.02
(1,1120)	1:A:87:ALA:H	1:A:88:ARG:HG3	14	0.02
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	9	0.02
(1,1091)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	9	0.02
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	9	0.02
(1,1091)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	9	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD11	7	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD12	7	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD13	7	0.02
(1,1062)	1:A:81:ILE:HG21	1:A:83:GLY:H	3	0.02
(1,1062)	1:A:81:ILE:HG22	1:A:83:GLY:H	3	0.02
(1,1062)	1:A:81:ILE:HG23	1:A:83:GLY:H	3	0.02
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	4	0.02
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	4	0.02
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	4	0.02
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	10	0.02
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	10	0.02
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	10	0.02
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD2	20	0.02
(1,1044)	1:A:80:ARG:H	1:A:80:ARG:HD3	20	0.02
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	4	0.02
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE22	4	0.02
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	4	0.02
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE22	4	0.02
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	5	0.02
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	5	0.02
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	8	0.02
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	8	0.02
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	13	0.02
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	13	0.02
(1,1000)	1:A:74:GLY:HA2	1:A:75:THR:HB	14	0.02
(1,1000)	1:A:74:GLY:HA3	1:A:75:THR:HB	14	0.02
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	15	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	15	0.02
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	15	0.02
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	3	0.01
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	3	0.01
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	3	0.01
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	3	0.01
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	20	0.01
(1,993)	1:A:73:GLU:HB2	1:A:78:TYR:HE2	20	0.01
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE1	20	0.01
(1,993)	1:A:73:GLU:HB3	1:A:78:TYR:HE2	20	0.01
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	12	0.01
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	12	0.01
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	12	0.01
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG21	1:A:97:ALA:HB3	12	0.01
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG22	1:A:97:ALA:HB3	12	0.01
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB1	12	0.01
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB2	12	0.01
(1,99)	1:B:15:VAL:HG23	1:A:97:ALA:HB3	12	0.01
(1,978)	1:A:72:ARG:HA	1:A:77:GLN:HA	4	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD11	6	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD12	6	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD13	6	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	14	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	14	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	14	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	14	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	14	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	14	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	14	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	14	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH11	16	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH12	16	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH21	16	0.01
(1,968)	1:A:71:ARG:HD2	1:A:71:ARG:HH22	16	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH11	16	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH12	16	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH21	16	0.01
(1,968)	1:A:71:ARG:HD3	1:A:71:ARG:HH22	16	0.01
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	7	0.01
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	7	0.01
(1,942)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	7	0.01
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	11	0.01
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	11	0.01
(1,895)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	11	0.01
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	11	0.01
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	11	0.01
(1,895)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	11	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG11	2	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG12	2	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG13	2	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG11	5	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG12	5	0.01
(1,889)	1:A:67:LEU:HA	1:A:86:VAL:HG13	5	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	5	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	5	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	5	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	5	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	5	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	5	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	16	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	16	0.01
(1,883)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	16	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD21	16	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD22	16	0.01
(1,883)	1:A:66:GLY:HA3	1:A:67:LEU:HD23	16	0.01
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	12	0.01
(1,864)	1:A:63:LYS:HE2	1:A:79:TYR:HE2	12	0.01
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	12	0.01
(1,864)	1:A:63:LYS:HE3	1:A:79:TYR:HE2	12	0.01
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	9	0.01
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	9	0.01
(1,862)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	9	0.01
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	9	0.01
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,862)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	9	0.01
(1,852)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	14	0.01
(1,852)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	14	0.01
(1,852)	1:A:63:LYS:HB3	1:A:63:LYS:HE2	14	0.01
(1,852)	1:A:63:LYS:HB3	1:A:63:LYS:HE3	14	0.01
(1,843)	1:A:62:LEU:HD11	1:A:63:LYS:H	14	0.01
(1,843)	1:A:62:LEU:HD12	1:A:63:LYS:H	14	0.01
(1,843)	1:A:62:LEU:HD13	1:A:63:LYS:H	14	0.01
(1,843)	1:A:62:LEU:HD11	1:A:63:LYS:H	15	0.01
(1,843)	1:A:62:LEU:HD12	1:A:63:LYS:H	15	0.01
(1,843)	1:A:62:LEU:HD13	1:A:63:LYS:H	15	0.01
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	9	0.01
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	9	0.01
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	9	0.01
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG2	5	0.01
(1,817)	1:A:60:GLN:HA	1:A:63:LYS:HG3	5	0.01
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	12	0.01
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE22	12	0.01
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	12	0.01
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE22	12	0.01
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	12	0.01
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE22	12	0.01
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	7	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	7	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	7	0.01
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD11	3	0.01
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD12	3	0.01
(1,773)	1:A:56:SER:HA	1:A:59:LEU:HD13	3	0.01
(1,76)	1:B:12:LEU:HD21	1:A:28:LEU:HB2	13	0.01
(1,76)	1:B:12:LEU:HD21	1:A:28:LEU:HB3	13	0.01
(1,76)	1:B:12:LEU:HD22	1:A:28:LEU:HB2	13	0.01
(1,76)	1:B:12:LEU:HD22	1:A:28:LEU:HB3	13	0.01
(1,76)	1:B:12:LEU:HD23	1:A:28:LEU:HB2	13	0.01
(1,76)	1:B:12:LEU:HD23	1:A:28:LEU:HB3	13	0.01
(1,748)	1:A:53:THR:H	1:A:53:THR:HB	12	0.01
(1,747)	1:A:53:THR:HG21	1:A:54:THR:H	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,747)	1:A:53:THR:HG22	1:A:54:THR:H	8	0.01
(1,747)	1:A:53:THR:HG23	1:A:54:THR:H	8	0.01
(1,746)	1:A:53:THR:HB	1:A:55:ALA:H	15	0.01
(1,714)	1:A:50:MET:H	1:A:50:MET:HE1	10	0.01
(1,714)	1:A:50:MET:H	1:A:50:MET:HE2	10	0.01
(1,714)	1:A:50:MET:H	1:A:50:MET:HE3	10	0.01
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB1	11	0.01
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB2	11	0.01
(1,712)	1:A:50:MET:HG2	1:A:55:ALA:HB3	11	0.01
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB1	11	0.01
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB2	11	0.01
(1,712)	1:A:50:MET:HG3	1:A:55:ALA:HB3	11	0.01
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG21	1	0.01
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG22	1	0.01
(1,711)	1:A:50:MET:HG2	1:A:54:THR:HG23	1	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG21	1	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG22	1	0.01
(1,711)	1:A:50:MET:HG3	1:A:54:THR:HG23	1	0.01
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	6	0.01
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	6	0.01
(1,617)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	6	0.01
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	19	0.01
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	19	0.01
(1,614)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	19	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	3	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	3	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	3	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	3	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	3	0.01
(1,612)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	3	0.01
(1,612)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	3	0.01
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	14	0.01
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	14	0.01
(1,611)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	14	0.01
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB1	14	0.01
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB2	14	0.01
(1,611)	1:A:42:GLU:HG3	1:A:45:ALA:HB3	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	7	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD11	14	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD12	14	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD13	14	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD21	14	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD22	14	0.01
(1,604)	1:A:42:GLU:HA	1:A:52:LEU:HD23	14	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	5	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	5	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	5	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	5	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	5	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	5	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	5	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	5	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	5	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	17	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	17	0.01
(1,590)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	17	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	17	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	17	0.01
(1,590)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	17	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	17	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	17	0.01
(1,590)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	17	0.01
(1,541)	1:A:40:ALA:HA	1:A:78:TYR:HA	1	0.01
(1,541)	1:A:40:ALA:HA	1:A:78:TYR:HA	7	0.01
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD11	5	0.01
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD12	5	0.01
(1,498)	1:A:35:ALA:HA	1:A:81:ILE:HD13	5	0.01
(1,488)	1:A:34:LEU:HD21	1:A:37:GLY:H	9	0.01
(1,488)	1:A:34:LEU:HD22	1:A:37:GLY:H	9	0.01
(1,488)	1:A:34:LEU:HD23	1:A:37:GLY:H	9	0.01
(1,474)	1:A:33:LEU:HG	1:A:39:ARG:HE	17	0.01
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD11	7	0.01
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD12	7	0.01
(1,445)	1:A:31:LEU:H	1:A:62:LEU:HD13	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,433)	1:A:31:LEU:HD21	1:A:81:ILE:HA	16	0.01
(1,433)	1:A:31:LEU:HD22	1:A:81:ILE:HA	16	0.01
(1,433)	1:A:31:LEU:HD23	1:A:81:ILE:HA	16	0.01
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG11	5	0.01
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG12	5	0.01
(1,421)	1:A:31:LEU:HD11	1:A:86:VAL:HG13	5	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG11	5	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG12	5	0.01
(1,421)	1:A:31:LEU:HD12	1:A:86:VAL:HG13	5	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG11	5	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG12	5	0.01
(1,421)	1:A:31:LEU:HD13	1:A:86:VAL:HG13	5	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	2	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	13	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD11	5	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD12	5	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD13	5	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	6	0.01
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	6	0.01
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	6	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	6	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	6	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	6	0.01
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	16	0.01
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	16	0.01
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	16	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG21	16	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG22	16	0.01
(1,361)	1:A:29:GLN:HG3	1:A:48:THR:HG23	16	0.01
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE1	4	0.01
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE2	4	0.01
(1,357)	1:A:29:GLN:HE21	1:A:50:MET:HE3	4	0.01
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE1	4	0.01
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE2	4	0.01
(1,357)	1:A:29:GLN:HE22	1:A:50:MET:HE3	4	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	10	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	10	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	10	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	10	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	10	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	10	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE1	14	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE2	14	0.01
(1,356)	1:A:29:GLN:HB2	1:A:50:MET:HE3	14	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE1	14	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE2	14	0.01
(1,356)	1:A:29:GLN:HB3	1:A:50:MET:HE3	14	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	2	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	2	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	2	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	2	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	8	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	8	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	8	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	8	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE21	14	0.01
(1,352)	1:A:29:GLN:HB2	1:A:29:GLN:HE22	14	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE21	14	0.01
(1,352)	1:A:29:GLN:HB3	1:A:29:GLN:HE22	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE1	4	0.01
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE2	4	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE1	4	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE2	4	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE1	4	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE2	4	0.01
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	19	0.01
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	19	0.01
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	19	0.01
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE1	20	0.01
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE2	20	0.01
(1,324)	1:A:27:ARG:HA	1:A:50:MET:HE3	20	0.01
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	11	0.01
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	11	0.01
(1,313)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	11	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	14	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	14	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	14	0.01
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	7	0.01
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	7	0.01
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	7	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	8	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	8	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	8	0.01
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	8	0.01
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	8	0.01
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	8	0.01
(1,278)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	15	0.01
(1,278)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	15	0.01
(1,278)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	15	0.01
(1,277)	1:A:21:ALA:HB1	1:A:65:GLY:HA3	2	0.01
(1,277)	1:A:21:ALA:HB2	1:A:65:GLY:HA3	2	0.01
(1,277)	1:A:21:ALA:HB3	1:A:65:GLY:HA3	2	0.01
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	1	0.01
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	1	0.01
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	1	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD11	1	0.01
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD12	1	0.01
(1,27)	1:A:14:GLN:HG3	1:B:101:LEU:HD13	1	0.01
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	4	0.01
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	9	0.01
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	14	0.01
(1,2607)	1:B:97:ALA:H	1:B:93:VAL:O	17	0.01
(1,2601)	1:B:94:GLN:H	1:B:90:PHE:O	5	0.01
(1,2601)	1:B:94:GLN:H	1:B:90:PHE:O	9	0.01
(1,2601)	1:B:94:GLN:H	1:B:90:PHE:O	14	0.01
(1,2591)	1:B:89:LEU:H	1:B:85:ASP:O	1	0.01
(1,2591)	1:B:89:LEU:H	1:B:85:ASP:O	3	0.01
(1,2591)	1:B:89:LEU:H	1:B:85:ASP:O	6	0.01
(1,2587)	1:B:87:ALA:H	1:B:83:GLY:O	13	0.01
(1,2583)	1:B:80:ARG:H	1:B:69:GLU:O	1	0.01
(1,2583)	1:B:80:ARG:H	1:B:69:GLU:O	5	0.01
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	2	0.01
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	7	0.01
(1,2577)	1:B:76:ARG:H	1:B:73:GLU:O	15	0.01
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	4	0.01
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	6	0.01
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	11	0.01
(1,2573)	1:B:71:ARG:H	1:B:78:TYR:O	12	0.01
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	1	0.01
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	6	0.01
(1,2567)	1:B:66:GLY:H	1:B:63:LYS:O	16	0.01
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	4	0.01
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	10	0.01
(1,2565)	1:B:65:GLY:H	1:B:61:ALA:O	17	0.01
(1,2561)	1:B:63:LYS:H	1:B:59:LEU:O	3	0.01
(1,2559)	1:B:62:LEU:H	1:B:58:ASN:O	7	0.01
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	5	0.01
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	9	0.01
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	10	0.01
(1,2557)	1:B:61:ALA:H	1:B:57:ALA:O	16	0.01
(1,2555)	1:B:60:GLN:H	1:B:56:SER:O	3	0.01
(1,2551)	1:B:58:ASN:H	1:B:54:THR:O	6	0.01
(1,2551)	1:B:58:ASN:H	1:B:54:THR:O	14	0.01
(1,2549)	1:B:57:ALA:H	1:B:53:THR:O	8	0.01
(1,2549)	1:B:57:ALA:H	1:B:53:THR:O	9	0.01
(1,2549)	1:B:57:ALA:H	1:B:53:THR:O	16	0.01
(1,2543)	1:B:50:MET:H	1:B:45:ALA:O	18	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	2	0.01
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	11	0.01
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	14	0.01
(1,2541)	1:B:49:GLY:H	1:B:46:THR:O	15	0.01
(1,2539)	1:B:48:THR:H	1:B:44:ILE:O	4	0.01
(1,2539)	1:B:48:THR:H	1:B:44:ILE:O	7	0.01
(1,2535)	1:B:46:THR:H	1:B:42:GLU:O	16	0.01
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	1	0.01
(1,2529)	1:B:41:VAL:H	1:B:77:GLN:O	18	0.01
(1,2528)	1:B:39:ARG:N	1:B:79:TYR:O	19	0.01
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	3	0.01
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	4	0.01
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	13	0.01
(1,2527)	1:B:39:ARG:H	1:B:79:TYR:O	20	0.01
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	3	0.01
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	6	0.01
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	12	0.01
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	13	0.01
(1,2525)	1:B:35:ALA:H	1:B:31:LEU:O	15	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	5	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	8	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	14	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	16	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	19	0.01
(1,2521)	1:B:33:LEU:H	1:B:29:GLN:O	20	0.01
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	6	0.01
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	14	0.01
(1,2517)	1:B:22:LEU:H	1:B:18:VAL:O	15	0.01
(1,2515)	1:B:21:ALA:H	1:B:17:ARG:O	17	0.01
(1,2511)	1:B:19:GLY:H	1:B:15:VAL:O	5	0.01
(1,2511)	1:B:19:GLY:H	1:B:15:VAL:O	7	0.01
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	13	0.01
(1,2509)	1:B:18:VAL:H	1:B:14:GLN:O	16	0.01
(1,2507)	1:B:17:ARG:H	1:B:13:ASP:O	15	0.01
(1,2505)	1:B:16:ALA:H	1:B:12:LEU:O	6	0.01
(1,2505)	1:B:16:ALA:H	1:B:12:LEU:O	8	0.01
(1,2502)	1:B:14:GLN:N	1:B:10:ALA:O	9	0.01
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	3	0.01
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	4	0.01
(1,2501)	1:B:14:GLN:H	1:B:10:ALA:O	20	0.01
(1,2495)	1:A:98:ASP:H	1:A:94:GLN:O	12	0.01
(1,2493)	1:A:97:ALA:H	1:A:93:VAL:O	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	13	0.01
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	14	0.01
(1,2487)	1:A:94:GLN:H	1:A:90:PHE:O	16	0.01
(1,2479)	1:A:90:PHE:H	1:A:86:VAL:O	17	0.01
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	1	0.01
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	6	0.01
(1,2477)	1:A:89:LEU:H	1:A:85:ASP:O	13	0.01
(1,2473)	1:A:87:ALA:H	1:A:83:GLY:O	3	0.01
(1,2473)	1:A:87:ALA:H	1:A:83:GLY:O	8	0.01
(1,2469)	1:A:80:ARG:H	1:A:69:GLU:O	16	0.01
(1,2469)	1:A:80:ARG:H	1:A:69:GLU:O	20	0.01
(1,2465)	1:A:78:TYR:H	1:A:71:ARG:O	16	0.01
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	6	0.01
(1,2463)	1:A:76:ARG:H	1:A:73:GLU:O	10	0.01
(1,2459)	1:A:71:ARG:H	1:A:78:TYR:O	18	0.01
(1,2459)	1:A:71:ARG:H	1:A:78:TYR:O	19	0.01
(1,2456)	1:A:67:LEU:N	1:A:62:LEU:O	12	0.01
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	1	0.01
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	3	0.01
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	11	0.01
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	16	0.01
(1,2453)	1:A:66:GLY:H	1:A:63:LYS:O	17	0.01
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	2	0.01
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	6	0.01
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	13	0.01
(1,2451)	1:A:65:GLY:H	1:A:61:ALA:O	18	0.01
(1,2445)	1:A:62:LEU:H	1:A:58:ASN:O	13	0.01
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	4	0.01
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	7	0.01
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	14	0.01
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	15	0.01
(1,2443)	1:A:61:ALA:H	1:A:57:ALA:O	17	0.01
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	3	0.01
(1,2437)	1:A:58:ASN:H	1:A:54:THR:O	5	0.01
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	3	0.01
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	12	0.01
(1,2435)	1:A:57:ALA:H	1:A:53:THR:O	16	0.01
(1,2429)	1:A:50:MET:H	1:A:45:ALA:O	11	0.01
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	6	0.01
(1,2427)	1:A:49:GLY:H	1:A:46:THR:O	8	0.01
(1,2425)	1:A:48:THR:H	1:A:44:ILE:O	5	0.01
(1,2425)	1:A:48:THR:H	1:A:44:ILE:O	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2421)	1:A:46:THR:H	1:A:42:GLU:O	2	0.01
(1,2421)	1:A:46:THR:H	1:A:42:GLU:O	14	0.01
(1,2421)	1:A:46:THR:H	1:A:42:GLU:O	19	0.01
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	9	0.01
(1,2415)	1:A:41:VAL:H	1:A:77:GLN:O	12	0.01
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	2	0.01
(1,2413)	1:A:39:ARG:H	1:A:79:TYR:O	3	0.01
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	12	0.01
(1,2411)	1:A:35:ALA:H	1:A:31:LEU:O	14	0.01
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	2	0.01
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	8	0.01
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	12	0.01
(1,2407)	1:A:33:LEU:H	1:A:29:GLN:O	14	0.01
(1,2403)	1:A:22:LEU:H	1:A:18:VAL:O	8	0.01
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	6	0.01
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	10	0.01
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	11	0.01
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	19	0.01
(1,2401)	1:A:21:ALA:H	1:A:17:ARG:O	20	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	12	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	12	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	12	0.01
(1,2399)	1:A:20:LYS:H	1:A:16:ALA:O	11	0.01
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	3	0.01
(1,2395)	1:A:18:VAL:H	1:A:14:GLN:O	20	0.01
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	3	0.01
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	6	0.01
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	8	0.01
(1,2393)	1:A:17:ARG:H	1:A:13:ASP:O	11	0.01
(1,2391)	1:A:16:ALA:H	1:A:12:LEU:O	8	0.01
(1,2391)	1:A:16:ALA:H	1:A:12:LEU:O	20	0.01
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	1	0.01
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	4	0.01
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	18	0.01
(1,2387)	1:A:14:GLN:H	1:A:10:ALA:O	19	0.01
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	4	0.01
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	8	0.01
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	12	0.01
(1,2385)	1:A:11:LEU:H	1:A:8:LYS:O	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2373)	1:B:100:HIS:H	1:B:100:HIS:HD2	18	0.01
(1,2351)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	4	0.01
(1,2351)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	4	0.01
(1,2351)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	4	0.01
(1,2350)	1:B:96:VAL:HG21	1:B:97:ALA:H	17	0.01
(1,2350)	1:B:96:VAL:HG22	1:B:97:ALA:H	17	0.01
(1,2350)	1:B:96:VAL:HG23	1:B:97:ALA:H	17	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	2	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	2	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	2	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	2	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	16	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	16	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	16	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	16	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE21	19	0.01
(1,2319)	1:B:94:GLN:HB2	1:B:94:GLN:HE22	19	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE21	19	0.01
(1,2319)	1:B:94:GLN:HB3	1:B:94:GLN:HE22	19	0.01
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG11	18	0.01
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG12	18	0.01
(1,2271)	1:B:89:LEU:HD21	1:B:93:VAL:HG13	18	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG11	18	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG12	18	0.01
(1,2271)	1:B:89:LEU:HD22	1:B:93:VAL:HG13	18	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG11	18	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG12	18	0.01
(1,2271)	1:B:89:LEU:HD23	1:B:93:VAL:HG13	18	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD21	6	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD22	6	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD23	6	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD21	10	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD22	10	0.01
(1,2263)	1:B:89:LEU:HA	1:B:92:LEU:HD23	10	0.01
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	18	0.01
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG3	18	0.01
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	8	0.01
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG3	8	0.01
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	7	0.01
(1,2162)	1:B:77:GLN:HG2	1:B:79:TYR:HE2	7	0.01
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE1	7	0.01
(1,2162)	1:B:77:GLN:HG3	1:B:79:TYR:HE2	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	2	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	2	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	2	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	2	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	5	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	5	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	5	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	5	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	9	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	9	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	9	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	9	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	17	0.01
(1,2157)	1:B:77:GLN:HB2	1:B:77:GLN:HE22	17	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	17	0.01
(1,2157)	1:B:77:GLN:HB3	1:B:77:GLN:HE22	17	0.01
(1,2146)	1:B:76:ARG:HD2	1:B:77:GLN:H	14	0.01
(1,2146)	1:B:76:ARG:HD3	1:B:77:GLN:H	14	0.01
(1,2129)	1:B:74:GLY:HA2	1:B:75:THR:HB	11	0.01
(1,2129)	1:B:74:GLY:HA3	1:B:75:THR:HB	11	0.01
(1,2124)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	12	0.01
(1,2124)	1:B:73:GLU:HG2	1:B:78:TYR:HE2	12	0.01
(1,2124)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	12	0.01
(1,2124)	1:B:73:GLU:HG3	1:B:78:TYR:HE2	12	0.01
(1,2085)	1:B:70:ALA:HB1	1:B:77:GLN:HE21	13	0.01
(1,2085)	1:B:70:ALA:HB2	1:B:77:GLN:HE21	13	0.01
(1,2085)	1:B:70:ALA:HB3	1:B:77:GLN:HE21	13	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	1	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	1	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	1	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	4	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	4	0.01
(1,2071)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	4	0.01
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG11	9	0.01
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG12	9	0.01
(1,2048)	1:B:68:VAL:HG11	1:B:86:VAL:HG13	9	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG11	9	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG12	9	0.01
(1,2048)	1:B:68:VAL:HG12	1:B:86:VAL:HG13	9	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG11	9	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG12	9	0.01
(1,2048)	1:B:68:VAL:HG13	1:B:86:VAL:HG13	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG11	5	0.01
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG12	5	0.01
(1,2027)	1:B:67:LEU:HD11	1:B:86:VAL:HG13	5	0.01
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG11	5	0.01
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG12	5	0.01
(1,2027)	1:B:67:LEU:HD12	1:B:86:VAL:HG13	5	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG11	5	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG12	5	0.01
(1,2027)	1:B:67:LEU:HD13	1:B:86:VAL:HG13	5	0.01
(1,2026)	1:B:67:LEU:HD11	1:B:86:VAL:HA	10	0.01
(1,2026)	1:B:67:LEU:HD12	1:B:86:VAL:HA	10	0.01
(1,2026)	1:B:67:LEU:HD13	1:B:86:VAL:HA	10	0.01
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG11	7	0.01
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG12	7	0.01
(1,2018)	1:B:67:LEU:HA	1:B:86:VAL:HG13	7	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	2	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	2	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	12	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	12	0.01
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	9	0.01
(1,1993)	1:B:63:LYS:HE2	1:B:79:TYR:HE2	9	0.01
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	9	0.01
(1,1993)	1:B:63:LYS:HE3	1:B:79:TYR:HE2	9	0.01
(1,1990)	1:B:63:LYS:HE2	1:B:69:GLU:HA	20	0.01
(1,1990)	1:B:63:LYS:HE3	1:B:69:GLU:HA	20	0.01
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG2	11	0.01
(1,1946)	1:B:60:GLN:HA	1:B:63:LYS:HG3	11	0.01
(1,1943)	1:B:60:GLN:HA	1:B:60:GLN:HE21	20	0.01
(1,1943)	1:B:60:GLN:HA	1:B:60:GLN:HE22	20	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD11	18	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD12	18	0.01
(1,1902)	1:B:56:SER:HA	1:B:59:LEU:HD13	18	0.01
(1,1877)	1:B:53:THR:H	1:B:53:THR:HB	17	0.01
(1,1874)	1:B:53:THR:HB	1:B:54:THR:H	14	0.01
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB1	10	0.01
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB2	10	0.01
(1,1841)	1:B:50:MET:HG2	1:B:55:ALA:HB3	10	0.01
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB1	10	0.01
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB2	10	0.01
(1,1841)	1:B:50:MET:HG3	1:B:55:ALA:HB3	10	0.01
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	11	0.01
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	11	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	11	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	1	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	1	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	1	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	5	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	5	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	5	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	7	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	7	0.01
(1,1743)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	7	0.01
(1,1742)	1:B:42:GLU:HG2	1:B:52:LEU:HG	20	0.01
(1,1742)	1:B:42:GLU:HG3	1:B:52:LEU:HG	20	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD11	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD12	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD13	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD21	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD22	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD23	10	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD11	13	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD12	13	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD13	13	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD21	13	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD22	13	0.01
(1,1733)	1:B:42:GLU:HA	1:B:52:LEU:HD23	13	0.01
(1,1723)	1:B:41:VAL:HG21	1:B:79:TYR:HE1	2	0.01
(1,1723)	1:B:41:VAL:HG21	1:B:79:TYR:HE2	2	0.01
(1,1723)	1:B:41:VAL:HG22	1:B:79:TYR:HE1	2	0.01
(1,1723)	1:B:41:VAL:HG22	1:B:79:TYR:HE2	2	0.01
(1,1723)	1:B:41:VAL:HG23	1:B:79:TYR:HE1	2	0.01
(1,1723)	1:B:41:VAL:HG23	1:B:79:TYR:HE2	2	0.01
(1,1722)	1:B:41:VAL:HG21	1:B:79:TYR:HD1	15	0.01
(1,1722)	1:B:41:VAL:HG21	1:B:79:TYR:HD2	15	0.01
(1,1722)	1:B:41:VAL:HG22	1:B:79:TYR:HD1	15	0.01
(1,1722)	1:B:41:VAL:HG22	1:B:79:TYR:HD2	15	0.01
(1,1722)	1:B:41:VAL:HG23	1:B:79:TYR:HD1	15	0.01
(1,1722)	1:B:41:VAL:HG23	1:B:79:TYR:HD2	15	0.01
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	14	0.01
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	14	0.01
(1,1719)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	14	0.01
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	14	0.01
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	14	0.01
(1,1719)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	14	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	14	0.01
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	14	0.01
(1,1719)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	14	0.01
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE1	6	0.01
(1,1701)	1:B:41:VAL:HB	1:B:79:TYR:HE2	6	0.01
(1,1676)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	1	0.01
(1,1676)	1:B:40:ALA:HB1	1:B:42:GLU:HG3	1	0.01
(1,1676)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	1	0.01
(1,1676)	1:B:40:ALA:HB2	1:B:42:GLU:HG3	1	0.01
(1,1676)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	1	0.01
(1,1676)	1:B:40:ALA:HB3	1:B:42:GLU:HG3	1	0.01
(1,1670)	1:B:40:ALA:HA	1:B:78:TYR:HA	8	0.01
(1,1657)	1:B:39:ARG:HA	1:B:39:ARG:HD2	15	0.01
(1,1657)	1:B:39:ARG:HA	1:B:39:ARG:HD3	15	0.01
(1,1620)	1:B:34:LEU:HD21	1:B:80:ARG:HA	4	0.01
(1,1620)	1:B:34:LEU:HD22	1:B:80:ARG:HA	4	0.01
(1,1620)	1:B:34:LEU:HD23	1:B:80:ARG:HA	4	0.01
(1,1616)	1:B:34:LEU:HD11	1:B:80:ARG:HA	8	0.01
(1,1616)	1:B:34:LEU:HD12	1:B:80:ARG:HA	8	0.01
(1,1616)	1:B:34:LEU:HD13	1:B:80:ARG:HA	8	0.01
(1,1587)	1:B:33:LEU:HA	1:B:36:GLN:HE21	14	0.01
(1,1587)	1:B:33:LEU:HA	1:B:36:GLN:HE22	14	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	4	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	4	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	4	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	4	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	4	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	4	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	10	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	10	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	10	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	10	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	10	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	10	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	15	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	15	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	15	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	15	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	15	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	15	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	20	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	20	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	20	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	20	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	20	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	10	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	10	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	10	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	10	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	10	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	10	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	10	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	10	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	10	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	20	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	20	0.01
(1,1563)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	20	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	20	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	20	0.01
(1,1563)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	20	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	20	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	20	0.01
(1,1563)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	20	0.01
(1,1549)	1:B:31:LEU:HD11	1:B:67:LEU:HG	14	0.01
(1,1549)	1:B:31:LEU:HD12	1:B:67:LEU:HG	14	0.01
(1,1549)	1:B:31:LEU:HD13	1:B:67:LEU:HG	14	0.01
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE1	11	0.01
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE2	11	0.01
(1,1486)	1:B:29:GLN:HE21	1:B:50:MET:HE3	11	0.01
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE1	11	0.01
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE2	11	0.01
(1,1486)	1:B:29:GLN:HE22	1:B:50:MET:HE3	11	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	1	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	1	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	1	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	1	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	1	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	1	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	4	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	4	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	4	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	4	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	4	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	4	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE1	6	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE2	6	0.01
(1,1485)	1:B:29:GLN:HB2	1:B:50:MET:HE3	6	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE1	6	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE2	6	0.01
(1,1485)	1:B:29:GLN:HB3	1:B:50:MET:HE3	6	0.01
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	19	0.01
(1,1481)	1:B:29:GLN:HB2	1:B:29:GLN:HE22	19	0.01
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE21	19	0.01
(1,1481)	1:B:29:GLN:HB3	1:B:29:GLN:HE22	19	0.01
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	2	0.01
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	2	0.01
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	2	0.01
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	2	0.01
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	2	0.01
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	2	0.01
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	12	0.01
(1,1466)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	12	0.01
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	12	0.01
(1,1466)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	12	0.01
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	12	0.01
(1,1466)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	12	0.01
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	6	0.01
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	6	0.01
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	10	0.01
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	10	0.01
(1,1458)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	10	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB1	10	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB2	10	0.01
(1,1458)	1:B:27:ARG:HD3	1:B:61:ALA:HB3	10	0.01
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE1	13	0.01
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE2	13	0.01
(1,1453)	1:B:27:ARG:HA	1:B:50:MET:HE3	13	0.01
(1,1447)	1:B:26:ARG:HA	1:B:29:GLN:HG2	13	0.01
(1,1447)	1:B:26:ARG:HA	1:B:29:GLN:HG3	13	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	7	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	7	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	7	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD11	15	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD12	15	0.01
(1,1439)	1:B:24:ASN:H	1:B:28:LEU:HD13	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	10	0.01
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	10	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	10	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	10	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	10	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	10	0.01
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	19	0.01
(1,1429)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	19	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	19	0.01
(1,1429)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	19	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	19	0.01
(1,1429)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	19	0.01
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	12	0.01
(1,141)	1:A:7:ARG:HB3	1:A:8:LYS:H	12	0.01
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	15	0.01
(1,141)	1:A:7:ARG:HB3	1:A:8:LYS:H	15	0.01
(1,1408)	1:B:21:ALA:HB1	1:B:65:GLY:H	19	0.01
(1,1408)	1:B:21:ALA:HB2	1:B:65:GLY:H	19	0.01
(1,1408)	1:B:21:ALA:HB3	1:B:65:GLY:H	19	0.01
(1,1407)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	3	0.01
(1,1407)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	3	0.01
(1,1407)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	3	0.01
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB2	19	0.01
(1,1364)	1:B:17:ARG:HD2	1:B:64:SER:HB3	19	0.01
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB2	19	0.01
(1,1364)	1:B:17:ARG:HD3	1:B:64:SER:HB3	19	0.01
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG2	18	0.01
(1,1355)	1:B:17:ARG:HA	1:B:20:LYS:HG3	18	0.01
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	2	0.01
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	2	0.01
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	2	0.01
(1,1284)	1:B:8:LYS:H	1:B:8:LYS:HG2	18	0.01
(1,1284)	1:B:8:LYS:H	1:B:8:LYS:HG3	18	0.01
(1,1279)	1:B:8:LYS:HB2	1:B:9:ALA:H	11	0.01
(1,1279)	1:B:8:LYS:HB3	1:B:9:ALA:H	11	0.01
(1,1259)	1:B:5:SER:HB2	1:B:6:ASP:H	19	0.01
(1,1259)	1:B:5:SER:HB3	1:B:6:ASP:H	19	0.01
(1,1249)	1:A:101:LEU:HD21	1:A:102:GLU:H	15	0.01
(1,1249)	1:A:101:LEU:HD22	1:A:102:GLU:H	15	0.01
(1,1249)	1:A:101:LEU:HD23	1:A:102:GLU:H	15	0.01
(1,1220)	1:A:96:VAL:HG11	1:A:100:HIS:HD2	2	0.01
(1,1220)	1:A:96:VAL:HG12	1:A:100:HIS:HD2	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1220)	1:A:96:VAL:HG13	1:A:100:HIS:HD2	2	0.01
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE21	6	0.01
(1,1190)	1:A:94:GLN:HB2	1:A:94:GLN:HE22	6	0.01
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE21	6	0.01
(1,1190)	1:A:94:GLN:HB3	1:A:94:GLN:HE22	6	0.01
(1,1180)	1:A:93:VAL:HG11	1:A:94:GLN:H	13	0.01
(1,1180)	1:A:93:VAL:HG12	1:A:94:GLN:H	13	0.01
(1,1180)	1:A:93:VAL:HG13	1:A:94:GLN:H	13	0.01
(1,1180)	1:A:93:VAL:HG11	1:A:94:GLN:H	18	0.01
(1,1180)	1:A:93:VAL:HG12	1:A:94:GLN:H	18	0.01
(1,1180)	1:A:93:VAL:HG13	1:A:94:GLN:H	18	0.01
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	1	0.01
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	1	0.01
(1,1156)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	1	0.01
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	1	0.01
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	1	0.01
(1,1156)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	1	0.01
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	10	0.01
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	10	0.01
(1,1152)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	10	0.01
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG11	10	0.01
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG12	10	0.01
(1,1152)	1:A:90:PHE:HB3	1:A:93:VAL:HG13	10	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	13	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	13	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	13	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD21	18	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD22	18	0.01
(1,1134)	1:A:89:LEU:HA	1:A:92:LEU:HD23	18	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB1	11	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB2	11	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB3	11	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB1	11	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB2	11	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB3	11	0.01
(1,1062)	1:A:81:ILE:HG21	1:A:83:GLY:H	7	0.01
(1,1062)	1:A:81:ILE:HG22	1:A:83:GLY:H	7	0.01
(1,1062)	1:A:81:ILE:HG23	1:A:83:GLY:H	7	0.01
(1,1062)	1:A:81:ILE:HG21	1:A:83:GLY:H	8	0.01
(1,1062)	1:A:81:ILE:HG22	1:A:83:GLY:H	8	0.01
(1,1062)	1:A:81:ILE:HG23	1:A:83:GLY:H	8	0.01
(1,1050)	1:A:81:ILE:HD11	1:A:82:ALA:H	20	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1050)	1:A:81:ILE:HD12	1:A:82:ALA:H	20	0.01
(1,1050)	1:A:81:ILE:HD13	1:A:82:ALA:H	20	0.01
(1,1035)	1:A:77:GLN:H	1:A:77:GLN:HG2	6	0.01
(1,1035)	1:A:77:GLN:H	1:A:77:GLN:HG3	6	0.01
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	1	0.01
(1,1028)	1:A:77:GLN:HB2	1:A:77:GLN:HE22	1	0.01
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	1	0.01
(1,1028)	1:A:77:GLN:HB3	1:A:77:GLN:HE22	1	0.01
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	2	0.01
(1,1018)	1:A:76:ARG:HD2	1:A:78:TYR:HE2	2	0.01
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	2	0.01
(1,1018)	1:A:76:ARG:HD3	1:A:78:TYR:HE2	2	0.01
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	7	0.01
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	7	0.01
(1,1017)	1:A:76:ARG:HD2	1:A:77:GLN:H	16	0.01
(1,1017)	1:A:76:ARG:HD3	1:A:77:GLN:H	16	0.01
(1,1000)	1:A:74:GLY:HA2	1:A:75:THR:HB	10	0.01
(1,1000)	1:A:74:GLY:HA3	1:A:75:THR:HB	10	0.01
(1,1000)	1:A:74:GLY:HA2	1:A:75:THR:HB	18	0.01
(1,1000)	1:A:74:GLY:HA3	1:A:75:THR:HB	18	0.01
(1,1000)	1:A:74:GLY:HA2	1:A:75:THR:HB	20	0.01
(1,1000)	1:A:74:GLY:HA3	1:A:75:THR:HB	20	0.01
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	9	0.01
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	9	0.01
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	9	0.01

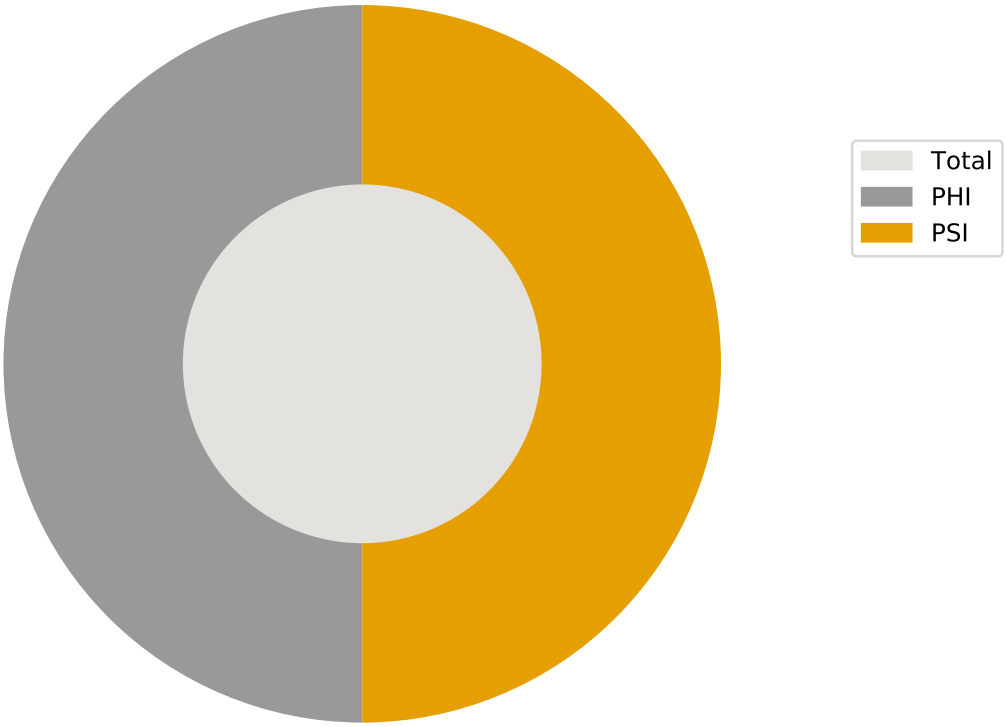
9 Dihedral angle restraints analysis

9.1 Dihedral angle restraints summary

Angle name	Count	%
PHI	168	50.0
PSI	168	50.0
Total	336	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	21	12.5	33.3
PSI	42	25.0	66.7

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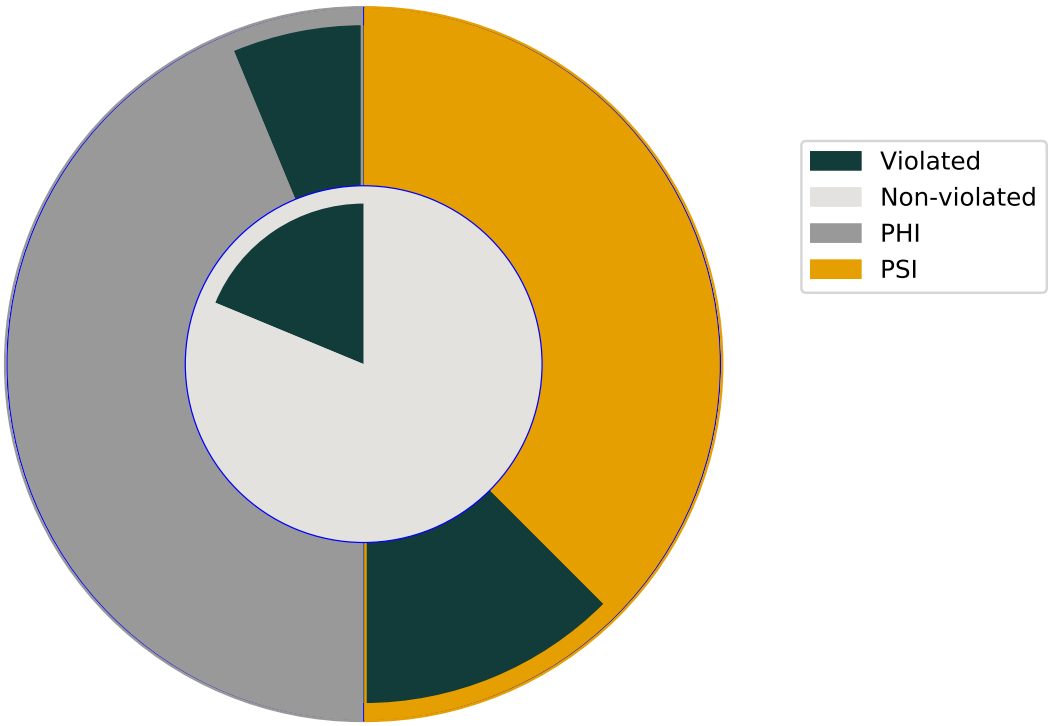
Angle name	Count	%[1]	%[2]
Total	63	18.8	100.0

[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



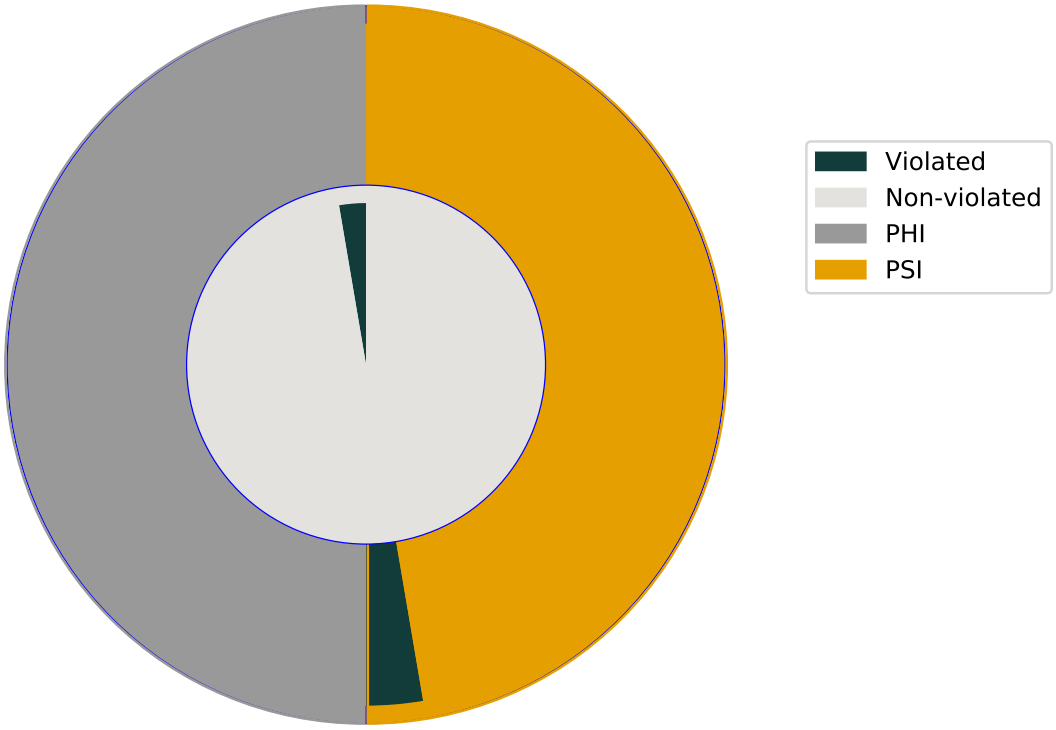
9.3 Consistent dihedral angle violations

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	9	5.4	100.0
Total	9	2.7	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	6.8	3.82
5.0-10.0	1.1	9.85
10.0-20.0	3.8	20.0
20.0-40.0	5.8	39.96
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	
10	16	26	1

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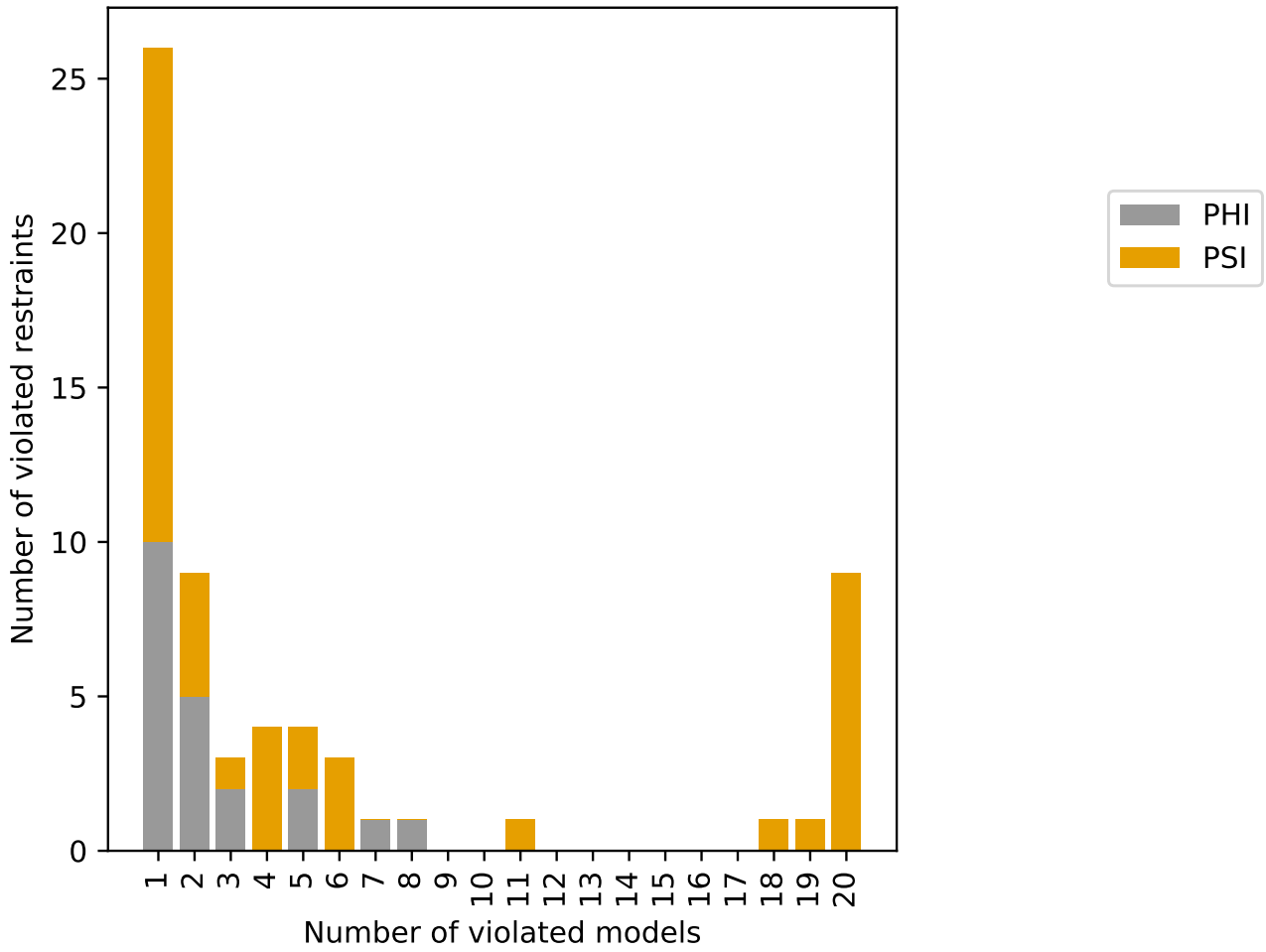
No. of violated restraints			No. of violated models
PHI	PSI	Total	
5	4	9	2
2	1	3	3
0	4	4	4
2	2	4	5
0	3	3	6
1	0	1	7
1	0	1	8
0	0	0	9
0	0	0	10
0	1	1	11
0	0	0	12
0	0	0	13
0	0	0	14
0	0	0	15
0	0	0	16
0	0	0	17
0	1	1	18
0	1	1	19
0	9	9	20

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	3	14	17	14.09	37.8
2	2	15	17	13.56	29.26
3	2	20	22	10.81	28.38
4	2	15	17	14.17	36.89
5	3	16	19	11.31	32.67
6	3	12	15	14.4	36.22
7	1	14	15	12.38	26.32
8	2	14	16	14.33	37.57
9	4	17	21	11.09	32.31

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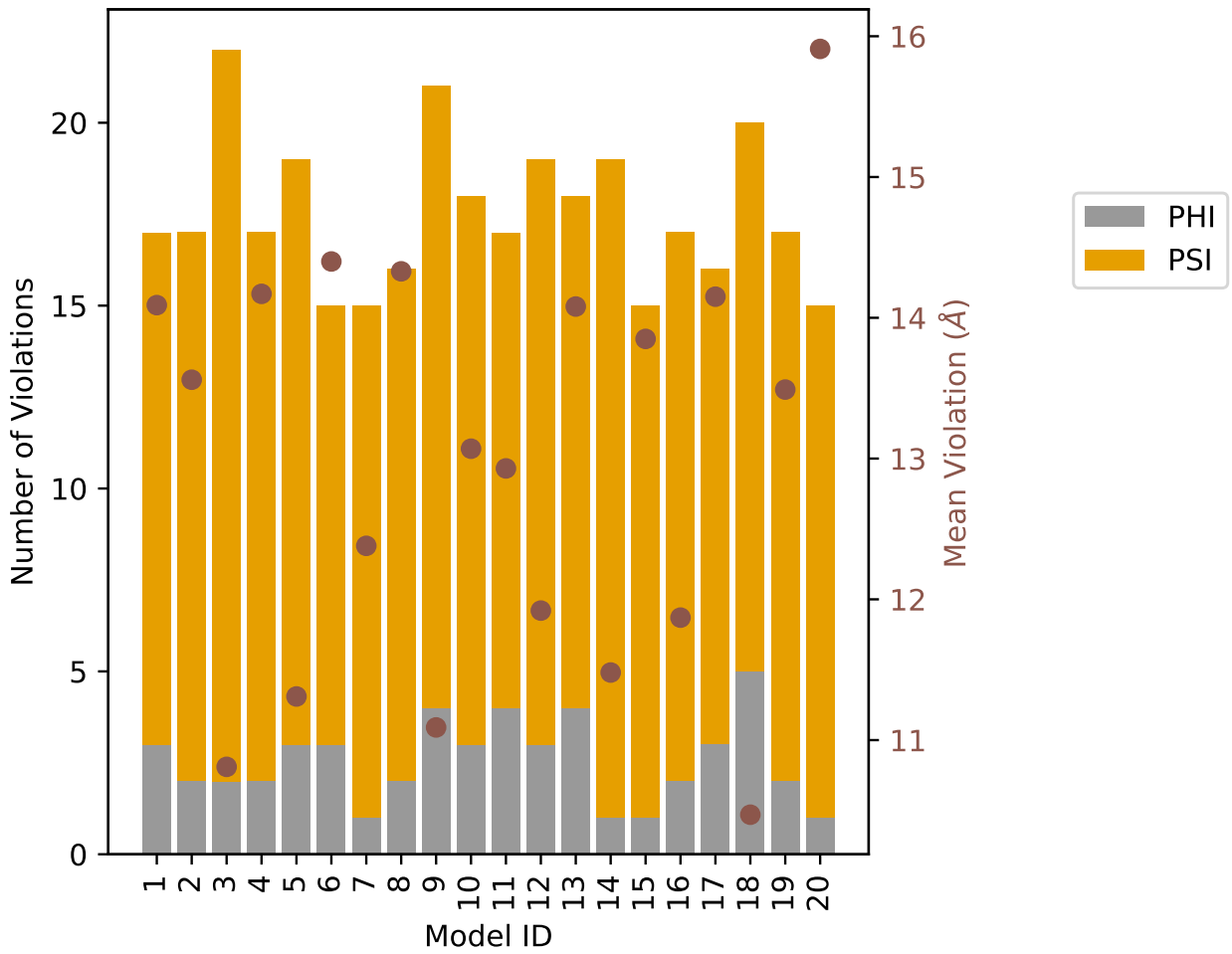
Model ID	No. of violations			Mean (∘)	Max (∘)
	PHI	PSI	Total		
10	3	15	18	13.07	29.69
11	4	13	17	12.93	37.74
12	3	16	19	11.92	38.81
13	4	14	18	14.08	30.17
14	1	18	19	11.48	39.96
15	1	14	15	13.85	26.41
16	2	15	17	11.87	34.79
17	3	13	16	14.15	35.48
18	5	15	20	10.47	29.69
19	2	15	17	13.49	29.54
20	1	14	15	15.91	29.18

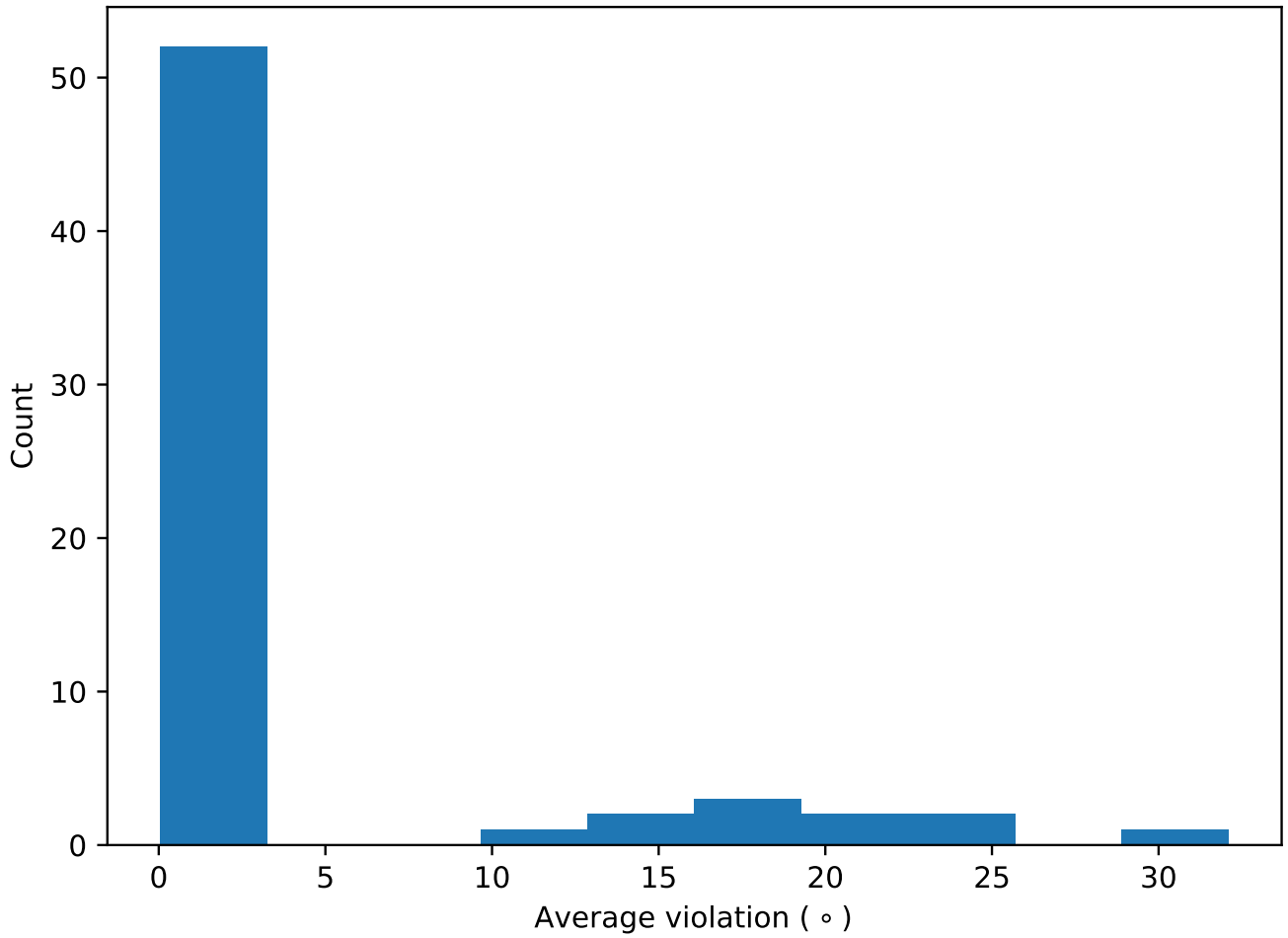
9.6.1 Bar graph : Violations in each model



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 (∘)
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	20	32.09	39.96
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	20	17.11	29.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	20	25.29	29.69
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	20	24.32	29.34
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	19	12.65	28.94
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	20	19.46	28.56
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	20	22.03	28.38
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	18	14.83	28.25
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	20	19.2	27.57
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	20	19.22	25.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (◦)	Max (◦)
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	20	15.63	21.87
(1,272)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:LYS:N	1	3.16	3.16
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	5	1.3	2.88
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	2	1.93	2.15
(1,274)	1:B:63:LYS:N	1:B:63:LYS:CA	1:B:63:LYS:C	1:B:64:SER:N	1	2.11	2.11
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	4	0.78	1.95
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	5	0.97	1.82
(1,222)	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1:B:37:GLY:N	1	1.75	1.75
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	3	0.96	1.65
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	4	0.77	1.63
(1,206)	1:B:28:LEU:N	1:B:28:LEU:CA	1:B:28:LEU:C	1:B:29:GLN:N	1	1.54	1.54
(1,202)	1:B:26:ARG:N	1:B:26:ARG:CA	1:B:26:ARG:C	1:B:27:ARG:N	1	1.5	1.5
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	2	1.39	1.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	11	0.59	1.37
(1,166)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:HIS:N	1	1.34	1.34
(1,284)	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	1:B:72:ARG:N	1	1.29	1.29
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	6	0.77	1.25
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	4	0.88	1.22
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	2	0.66	1.14
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	6	0.67	1.08
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	6	0.32	1.01
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	4	0.7	0.84
(1,170)	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1:B:8:LYS:N	1	0.77	0.77
(1,286)	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	1:B:73:GLU:N	1	0.74	0.74
(1,282)	1:B:70:ALA:N	1:B:70:ALA:CA	1:B:70:ALA:C	1:B:71:ARG:N	1	0.44	0.44
(1,164)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	1	0.44	0.44
(1,332)	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	1:B:99:GLU:N	1	0.37	0.37
(1,162)	1:A:97:ALA:N	1:A:97:ALA:CA	1:A:97:ALA:C	1:A:98:ASP:N	1	0.32	0.32
(1,288)	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1:B:74:GLY:N	1	0.31	0.31
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	2	0.19	0.21
(1,112)	1:A:69:GLU:N	1:A:69:GLU:CA	1:A:69:GLU:C	1:A:70:ALA:N	1	0.19	0.19
(1,334)	1:B:99:GLU:N	1:B:99:GLU:CA	1:B:99:GLU:C	1:B:100:HIS:N	1	0.18	0.18
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	7	0.79	1.81
(1,169)	1:B:6:ASP:C	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1	1.31	1.31
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	8	0.75	1.31
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	2	0.73	1.25
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	5	0.64	1.18
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	2	0.93	1.15
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	5	0.79	1.11
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	2	0.56	0.77
(1,123)	1:A:74:GLY:C	1:A:75:THR:N	1:A:75:THR:CA	1:A:75:THR:C	1	0.75	0.75
(1,297)	1:B:77:GLN:C	1:B:78:TYR:N	1:B:78:TYR:CA	1:B:78:TYR:C	1	0.71	0.71
(1,119)	1:A:72:ARG:C	1:A:73:GLU:N	1:A:73:GLU:CA	1:A:73:GLU:C	1	0.58	0.58
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	3	0.39	0.5
(1,287)	1:B:72:ARG:C	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1	0.47	0.47
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	3	0.29	0.47
(1,35)	1:A:26:ARG:C	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1	0.42	0.42
(1,221)	1:B:35:ALA:C	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1	0.41	0.41
(1,129)	1:A:77:GLN:C	1:A:78:TYR:N	1:A:78:TYR:CA	1:A:78:TYR:C	1	0.28	0.28
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	2	0.2	0.24
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	2	0.23	0.24

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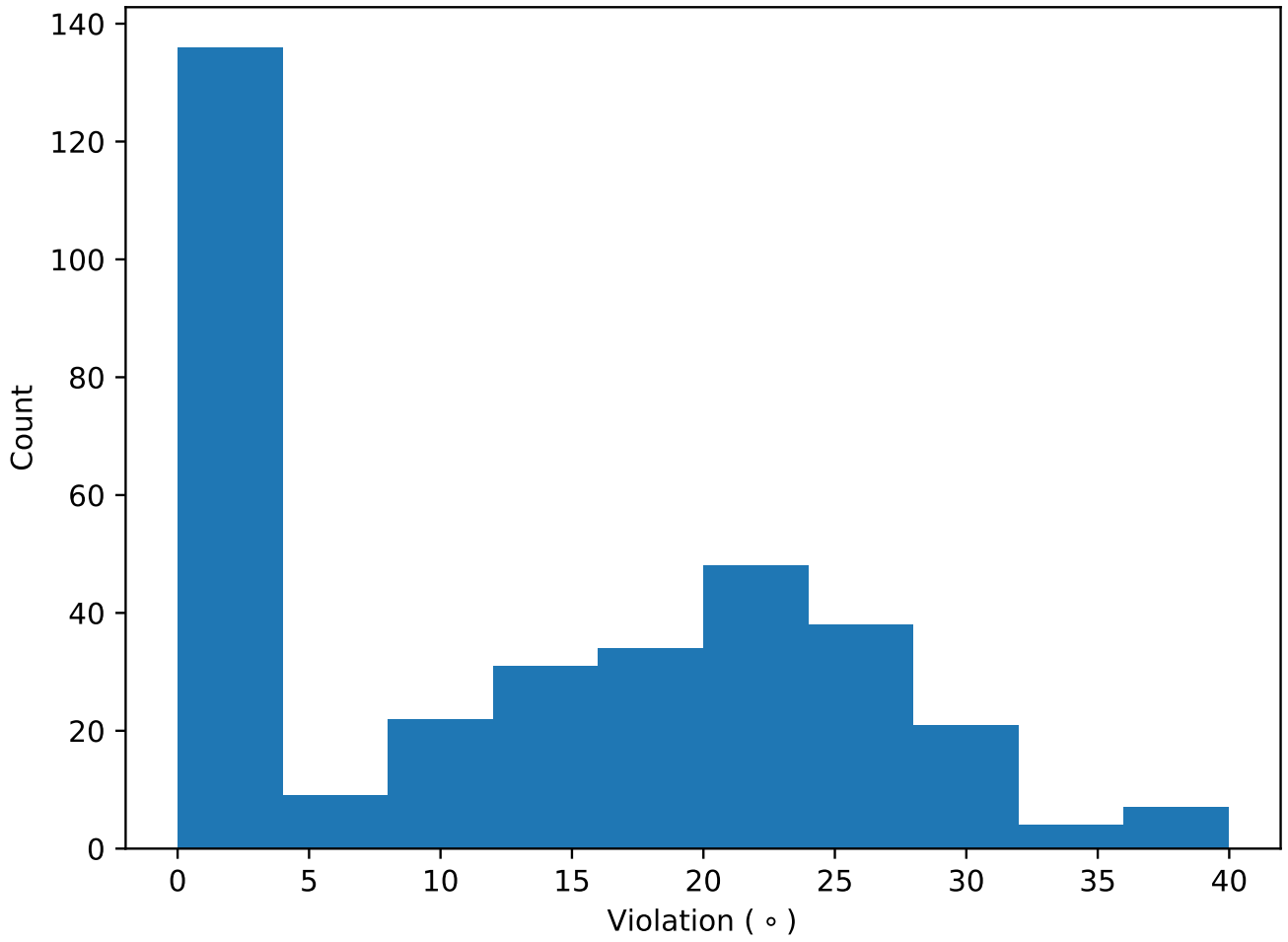
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean (∘)	Max (∘)
(1,117)	1:A:71:ARG:C	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1	0.07	0.07
(1,75)	1:A:47:ALA:C	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	1	0.06	0.06

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 (∘)
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	14	39.96
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	12	38.81
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	1	37.8
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	11	37.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	8	37.57
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	4	36.89
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	6	36.22
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	17	35.48
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	16	34.79
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	5	32.67
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	9	32.31
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	13	30.17
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	6	29.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	18	29.69
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	10	29.69
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	19	29.54
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	10	29.39
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	6	29.34
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	2	29.26
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	9	29.18
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	20	29.18
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	1	28.94
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	8	28.87
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	4	28.83
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	1	28.56
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	20	28.48
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	14	28.48
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	2	28.44
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	3	28.38
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	17	28.25
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	4	28.04
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	19	28.01
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	12	27.69
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	20	27.58
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	10	27.57
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	4	27.55
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	17	27.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	1	27.46
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	5	27.41
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	3	27.33
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	12	27.33
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	13	27.27
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	5	27.1
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	8	27.05
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	13	27.05
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	9	26.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	15	26.41
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	3	26.36
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	7	26.32
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	18	26.26
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	11	26.26
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	16	26.15
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	8	25.88
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	20	25.74
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	13	25.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	19	25.13
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	15	25.09
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	17	25.01
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	7	24.99
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	16	24.89
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	18	24.88
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	10	24.86
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	19	24.82
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	20	24.5
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	14	24.38
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	7	24.24
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	1	24.22
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	9	24.05
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	10	24.03
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	2	24.03
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	2	23.92
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	3	23.85
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	13	23.82
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	13	23.76
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	3	23.74
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	2	23.73
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	18	23.72
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	18	23.45
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	11	23.43
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	20	23.43
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	12	23.35
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	16	23.15
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	7	23.07
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	11	23.07
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	13	23.02
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	10	23.01
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	6	22.78
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	3	22.77
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	2	22.75
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	15	22.58
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	9	22.41
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	8	22.32
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	7	22.3
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	17	22.14
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	17	21.98
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	15	21.97
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	20	21.88
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	14	21.87
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	13	21.82
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	14	21.58
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	6	21.49
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	13	21.46
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	13	21.44
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	7	21.34
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	4	20.95
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	1	20.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	5	20.75
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	4	20.69
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	6	20.63
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	4	20.6
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	11	20.49
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	15	20.4
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	9	20.27
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	19	20.25
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	10	20.04
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	11	20.01
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	19	20.0
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	17	20.0
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	6	19.72
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	8	19.7
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	5	19.63
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	9	19.53
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	11	19.39
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	18	19.34
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	10	19.3
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	5	19.26
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	19	19.25
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	2	19.1
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	3	19.01
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	5	18.53
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	6	18.45
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	8	18.44
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	5	18.35
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	19	18.21
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	15	18.2
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	15	18.14
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	1	18.02
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	14	18.01
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	19	17.83
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	12	17.76
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	18	17.45
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	12	17.38
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	16	17.33
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	12	17.27
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	19	17.13
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	4	17.02
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	11	16.94
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	17	16.92
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	16	16.83
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	18	16.35
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	15	16.34
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	12	16.33
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	3	15.54
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	14	15.49
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	9	15.44
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	3	15.28
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	4	15.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	10	15.15
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	11	15.14
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	1	15.11
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	16	14.99
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	1	14.78
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	20	14.64
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	10	14.56
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	20	14.55
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	2	14.49
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	3	14.48
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	20	14.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	8	14.41
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	14	14.22
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	2	14.12
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	7	13.56
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	2	13.39
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	18	13.36
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	9	13.31
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	12	13.22
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	4	13.17
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	15	13.13
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	11	12.72
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	15	12.71
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	12	12.69
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	20	12.58
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	8	12.39
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	16	11.87
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	5	11.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	16	11.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	1	11.82
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	9	11.79
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	8	11.69
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	17	11.24
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	2	10.95
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	12	10.03
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	14	9.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	7	9.55
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	6	9.35
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	3	9.31
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	5	9.07
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	15	8.89
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	14	8.86
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	16	8.85
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	9	8.52
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	7	8.4
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	7	8.27
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	18	8.17
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	1	8.09
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	8	7.7
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	4	7.68
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	17	7.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	14	7.5
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	19	5.76
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	5	5.76
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	17	5.58
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	6	5.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	16	5.13
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	13	3.82
(1,272)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:LYS:N	3	3.16
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	3	2.88
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	10	2.83
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	7	2.48
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	14	2.15
(1,274)	1:B:63:LYS:N	1:B:63:LYS:CA	1:B:63:LYS:C	1:B:64:SER:N	3	2.11
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	13	1.95
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	2	1.82
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	12	1.81
(1,222)	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1:B:37:GLY:N	9	1.75
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	15	1.71
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	5	1.65
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	9	1.63
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	18	1.59
(1,206)	1:B:28:LEU:N	1:B:28:LEU:CA	1:B:28:LEU:C	1:B:29:GLN:N	9	1.54
(1,202)	1:B:26:ARG:N	1:B:26:ARG:CA	1:B:26:ARG:C	1:B:27:ARG:N	17	1.5
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	16	1.46
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	14	1.43
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	14	1.42
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	4	1.38
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	16	1.37
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	15	1.36
(1,166)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:HIS:N	3	1.34
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	10	1.32
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	10	1.31
(1,169)	1:B:6:ASP:C	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1	1.31
(1,284)	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	1:B:72:ARG:N	9	1.29
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	11	1.25
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	17	1.25
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	14	1.22
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	8	1.18
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	18	1.15
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	2	1.14
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	16	1.13
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	6	1.12
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	5	1.12
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	19	1.12
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	18	1.11
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	2	1.11
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	12	1.09
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	4	1.08
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	1	1.07
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	2	1.05
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	5	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	16	1.01
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	20	0.96
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	8	0.84
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	2	0.84
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	17	0.84
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	10	0.83
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	11	0.82
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	13	0.81
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	11	0.78
(1,170)	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1:B:8:LYS:N	18	0.77
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	6	0.77
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	9	0.75
(1,123)	1:A:74:GLY:C	1:A:75:THR:N	1:A:75:THR:CA	1:A:75:THR:C	17	0.75
(1,286)	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	1:B:73:GLU:N	10	0.74
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	4	0.72
(1,297)	1:B:77:GLN:C	1:B:78:TYR:N	1:B:78:TYR:CA	1:B:78:TYR:C	9	0.71
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	11	0.7
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	8	0.68
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	14	0.67
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	7	0.66
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	3	0.64
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	19	0.64
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	1	0.63
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	13	0.62
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	18	0.61
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	19	0.61
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	14	0.6
(1,119)	1:A:72:ARG:C	1:A:73:GLU:N	1:A:73:GLU:CA	1:A:73:GLU:C	16	0.58
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	4	0.5
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	18	0.49
(1,287)	1:B:72:ARG:C	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	11	0.47
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	9	0.47
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	11	0.46
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	12	0.46
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	19	0.44
(1,282)	1:B:70:ALA:N	1:B:70:ALA:CA	1:B:70:ALA:C	1:B:71:ARG:N	1	0.44
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	8	0.44
(1,164)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	12	0.44
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	3	0.44
(1,35)	1:A:26:ARG:C	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	10	0.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	3	0.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	9	0.42
(1,221)	1:B:35:ALA:C	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	6	0.41
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	16	0.4
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	2	0.4
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	15	0.4
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	15	0.39
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	9	0.37
(1,332)	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	1:B:99:GLU:N	4	0.37
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	20	0.37
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	19	0.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation (∘)
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	9	0.36
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	7	0.36
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	17	0.36
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	18	0.33
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	3	0.32
(1,162)	1:A:97:ALA:N	1:A:97:ALA:CA	1:A:97:ALA:C	1:A:98:ASP:N	6	0.32
(1,288)	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1:B:74:GLY:N	3	0.31
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	12	0.29
(1,129)	1:A:77:GLN:C	1:A:78:TYR:N	1:A:78:TYR:CA	1:A:78:TYR:C	18	0.28
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	14	0.26
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	13	0.26
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	14	0.24
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	13	0.24
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	12	0.23
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	5	0.23
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	13	0.22
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	13	0.21
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	12	0.21
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	5	0.21
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	1	0.2
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	18	0.2
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	10	0.19
(1,112)	1:A:69:GLU:N	1:A:69:GLU:CA	1:A:69:GLU:C	1:A:70:ALA:N	20	0.19
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	6	0.18
(1,334)	1:B:99:GLU:N	1:B:99:GLU:CA	1:B:99:GLU:C	1:B:100:HIS:N	18	0.18
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	4	0.17
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	8	0.16
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	19	0.16
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1	0.16
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	5	0.16
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	10	0.11
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	5	0.1
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	7	0.09
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	3	0.09
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	20	0.08
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	11	0.07
(1,117)	1:A:71:ARG:C	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	7	0.07
(1,75)	1:A:47:ALA:C	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	3	0.06
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	5	0.06
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	12	0.02