



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 2LRA / pdb_00002lra
BMRB ID : 18355
Title : NMR Structure of Signal Sequence Deleted (SSD) Rv0603 Protein from Mycobacterium tuberculosis without N-terminal His-tag
Authors : Tripathi, S.; Pulavarti, S.; Yadav, R.; Jain, A.; Pathak, P.; Meher, A.; Arora, A.
Deposited on : 2012-03-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

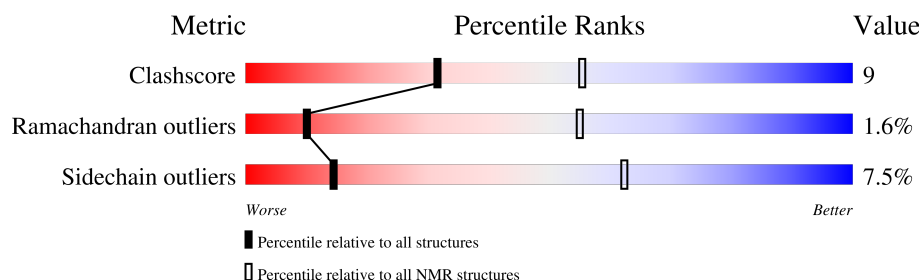
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	81	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:75 (73)	1.10	5

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. No single-model clusters were found.

Cluster number	Models
1	2, 5, 6, 7
2	1, 3, 4, 10
3	8, 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1110 atoms, of which 532 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POSSIBLE EXPORTED PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1110	346	532	102	129	1	

There are 5 discrepancies between the modelled and reference sequences:

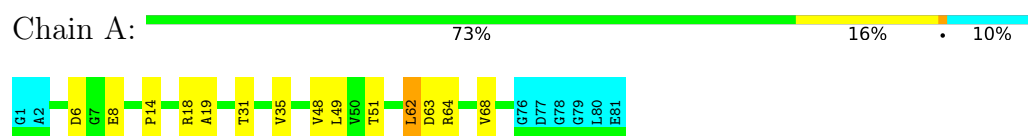
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O07775
A	2	ALA	-	expression tag	UNP O07775
A	3	MET	-	expression tag	UNP O07775
A	80	LEU	-	expression tag	UNP O07775
A	81	GLU	-	expression tag	UNP O07775

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: POSSIBLE EXPORTED PROTEIN

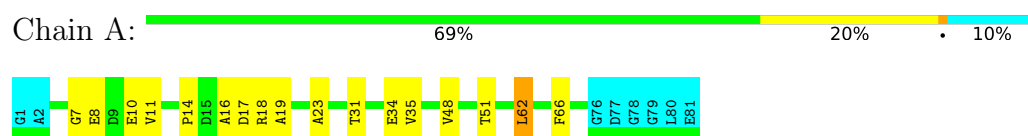


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

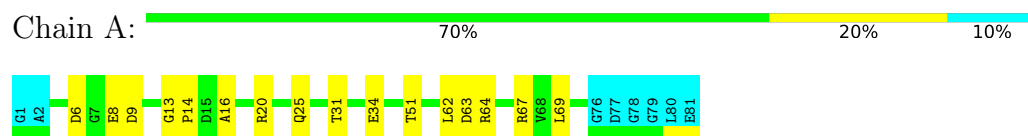
4.2.1 Score per residue for model 1

- Molecule 1: POSSIBLE EXPORTED PROTEIN



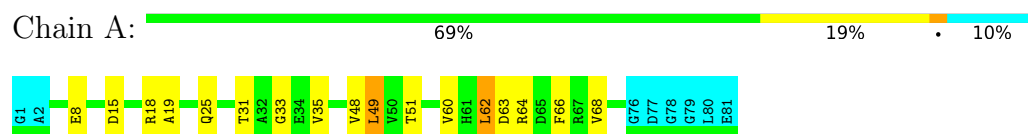
4.2.2 Score per residue for model 2

- Molecule 1: POSSIBLE EXPORTED PROTEIN



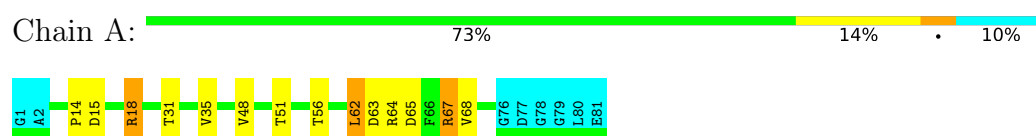
4.2.3 Score per residue for model 3

- Molecule 1: POSSIBLE EXPORTED PROTEIN



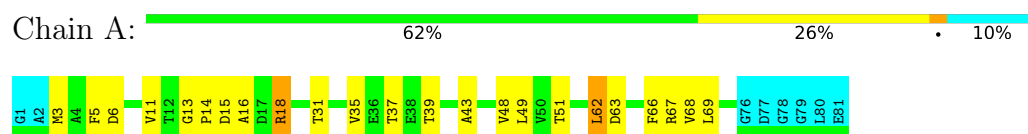
4.2.4 Score per residue for model 4

- Molecule 1: POSSIBLE EXPORTED PROTEIN



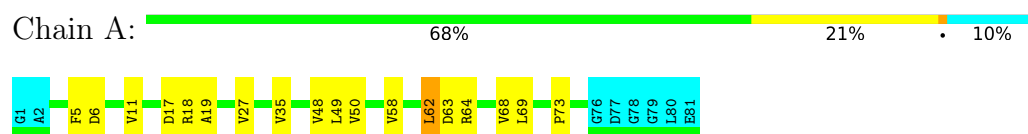
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: POSSIBLE EXPORTED PROTEIN



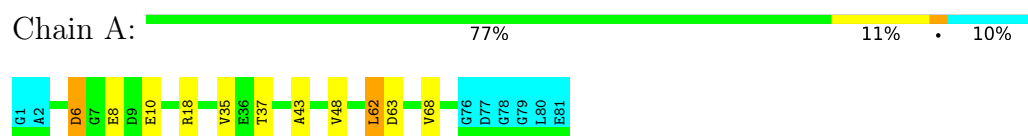
4.2.6 Score per residue for model 6

- Molecule 1: POSSIBLE EXPORTED PROTEIN



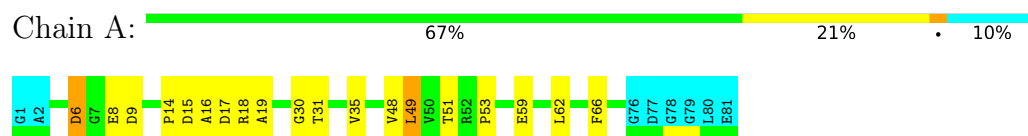
4.2.7 Score per residue for model 7

- Molecule 1: POSSIBLE EXPORTED PROTEIN



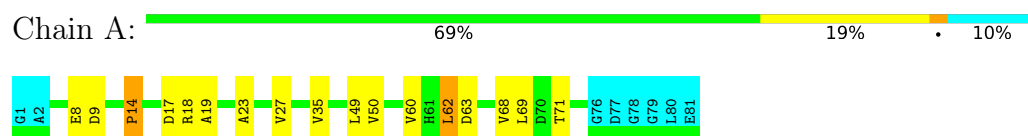
4.2.8 Score per residue for model 8

- Molecule 1: POSSIBLE EXPORTED PROTEIN



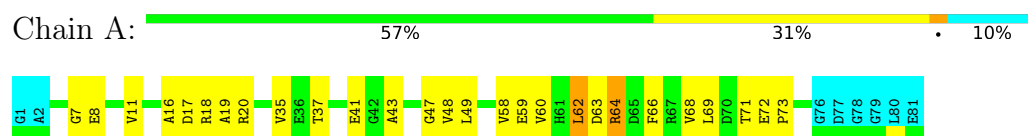
4.2.9 Score per residue for model 9

- Molecule 1: POSSIBLE EXPORTED PROTEIN



4.2.10 Score per residue for model 10

- Molecule 1: POSSIBLE EXPORTED PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *water refinement*.

Of the 200 calculated structures, 10 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
Cyana3.0	structure solution	
CNS	refinement	solve_1.21

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	865
Number of shifts mapped to atoms	865
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	531	492	491	9±2
All	All	5310	4920	4910	89

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ALA:HA	1:A:35:VAL:HG22	0.88	1.45	10	3
1:A:11:VAL:HG21	1:A:17:ASP:HB2	0.84	1.48	1	3
1:A:31:THR:HB	1:A:51:THR:HB	0.82	1.52	5	6
1:A:63:ASP:HB3	1:A:69:LEU:HD11	0.80	1.54	2	1
1:A:20:ARG:HD2	1:A:34:GLU:HG2	0.73	1.59	2	1
1:A:27:VAL:HB	1:A:50:VAL:HB	0.73	1.60	6	2
1:A:63:ASP:HB3	1:A:69:LEU:HD21	0.68	1.65	5	1
1:A:19:ALA:HB3	1:A:35:VAL:HG21	0.67	1.66	6	4
1:A:19:ALA:HB1	1:A:48:VAL:HG22	0.63	1.69	3	4
1:A:62:LEU:HD12	1:A:68:VAL:HA	0.62	1.71	5	7
1:A:35:VAL:HG11	1:A:48:VAL:HA	0.62	1.70	7	3
1:A:7:GLY:HA2	1:A:18:ARG:NH1	0.61	2.10	1	1
1:A:63:ASP:OD1	1:A:67:ARG:HB3	0.60	1.97	5	1
1:A:8:GLU:HG2	1:A:9:ASP:H	0.58	1.58	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:VAL:HB	1:A:60:VAL:HB	0.55	1.77	3	2
1:A:30:GLY:HA2	1:A:53:PRO:HD3	0.55	1.79	8	1
1:A:8:GLU:HG3	1:A:10:GLU:HG2	0.53	1.80	1	1
1:A:8:GLU:HG3	1:A:10:GLU:H	0.53	1.63	7	1
1:A:13:GLY:HA3	1:A:16:ALA:HB3	0.53	1.81	5	2
1:A:43:ALA:O	1:A:63:ASP:HA	0.53	2.05	10	2
1:A:18:ARG:HD2	1:A:18:ARG:H	0.52	1.64	4	1
1:A:18:ARG:HG2	1:A:18:ARG:HH11	0.51	1.66	7	1
1:A:19:ALA:HB2	1:A:66:PHE:HE1	0.50	1.66	1	2
1:A:49:LEU:H	1:A:49:LEU:HD23	0.49	1.67	8	1
1:A:15:ASP:O	1:A:18:ARG:HG2	0.49	2.08	8	1
1:A:5:PHE:HA	1:A:18:ARG:HD2	0.48	1.84	6	1
1:A:35:VAL:HB	1:A:47:GLY:O	0.47	2.09	10	1
1:A:15:ASP:HA	1:A:18:ARG:CG	0.47	2.40	3	1
1:A:7:GLY:HA2	1:A:17:ASP:OD1	0.47	2.09	10	1
1:A:6:ASP:H	1:A:18:ARG:HD3	0.47	1.68	7	1
1:A:58:VAL:HA	1:A:73:PRO:HA	0.47	1.85	6	2
1:A:6:ASP:N	1:A:18:ARG:HD2	0.47	2.24	8	1
1:A:6:ASP:O	1:A:18:ARG:HD2	0.47	2.10	5	1
1:A:15:ASP:HA	1:A:18:ARG:NE	0.47	2.25	5	1
1:A:63:ASP:HB2	1:A:69:LEU:HD21	0.46	1.87	9	3
1:A:16:ALA:HA	1:A:35:VAL:CG2	0.45	2.41	8	1
1:A:48:VAL:O	1:A:59:GLU:HA	0.45	2.11	8	2
1:A:15:ASP:HA	1:A:18:ARG:HG2	0.45	1.87	3	1
1:A:8:GLU:O	1:A:11:VAL:HG22	0.44	2.13	10	1
1:A:62:LEU:HD23	1:A:66:PHE:HD1	0.43	1.72	1	1
1:A:63:ASP:CG	1:A:64:ARG:N	0.43	2.77	3	3
1:A:35:VAL:CG1	1:A:48:VAL:HA	0.43	2.43	1	1
1:A:60:VAL:HG22	1:A:71:THR:HG23	0.42	1.91	9	1
1:A:3:MET:HB3	1:A:5:PHE:CE2	0.42	2.50	5	1
1:A:63:ASP:OD2	1:A:67:ARG:HB3	0.42	2.15	2	1
1:A:14:PRO:O	1:A:18:ARG:HG2	0.41	2.15	9	1
1:A:35:VAL:HG12	1:A:49:LEU:HG	0.41	1.90	5	1
1:A:33:GLY:HA3	1:A:49:LEU:HD11	0.41	1.91	3	1
1:A:60:VAL:HG22	1:A:71:THR:HG22	0.41	1.93	10	1
1:A:65:ASP:HB2	1:A:67:ARG:CZ	0.41	2.46	4	1
1:A:23:ALA:HB1	1:A:50:VAL:CG1	0.41	2.45	9	1
1:A:23:ALA:HB2	1:A:48:VAL:HG11	0.40	1.93	1	1
1:A:15:ASP:HA	1:A:18:ARG:HD3	0.40	1.93	4	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	73/81 (90%)	66±2 (90±3%)	6±2 (8±2%)	1±1 (2±1%)	10	55
All	All	730/810 (90%)	657 (90%)	61 (8%)	12 (2%)	10	55

All 4 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	14	PRO	6
1	A	6	ASP	4
1	A	11	VAL	1
1	A	43	ALA	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/55 (95%)	48±2 (92±3%)	4±2 (8±3%)	14	62
All	All	520/550 (95%)	481 (92%)	39 (8%)	14	62

All 16 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	62	LEU	10
1	A	49	LEU	5
1	A	64	ARG	3
1	A	66	PHE	3
1	A	18	ARG	3
1	A	37	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	25	GLN	2
1	A	17	ASP	2
1	A	34	GLU	1
1	A	8	GLU	1
1	A	56	THR	1
1	A	67	ARG	1
1	A	39	THR	1
1	A	20	ARG	1
1	A	41	GLU	1
1	A	72	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	865
Number of shifts mapped to atoms	865
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	-0.12 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	0.08 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	77	2.43 ± 0.14	Should be applied
^{15}N	75	-0.22 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 808 atoms were assigned a chemical shift out of a possible 890. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	365/366 (100%)	151/151 (100%)	145/146 (99%)	69/69 (100%)
Sidechain	411/487 (84%)	282/315 (90%)	128/153 (84%)	1/19 (5%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	32/37 (86%)	16/18 (89%)	16/17 (94%)	0/2 (0%)
Overall	808/890 (91%)	449/484 (93%)	289/316 (91%)	70/90 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 865 atoms were assigned a chemical shift out of a possible 962. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	399/410 (97%)	167/171 (98%)	157/162 (97%)	75/77 (97%)
Sidechain	434/515 (84%)	298/333 (89%)	135/163 (83%)	1/19 (5%)
Aromatic	32/37 (86%)	16/18 (89%)	16/17 (94%)	0/2 (0%)
Overall	865/962 (90%)	481/522 (92%)	308/342 (90%)	76/98 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

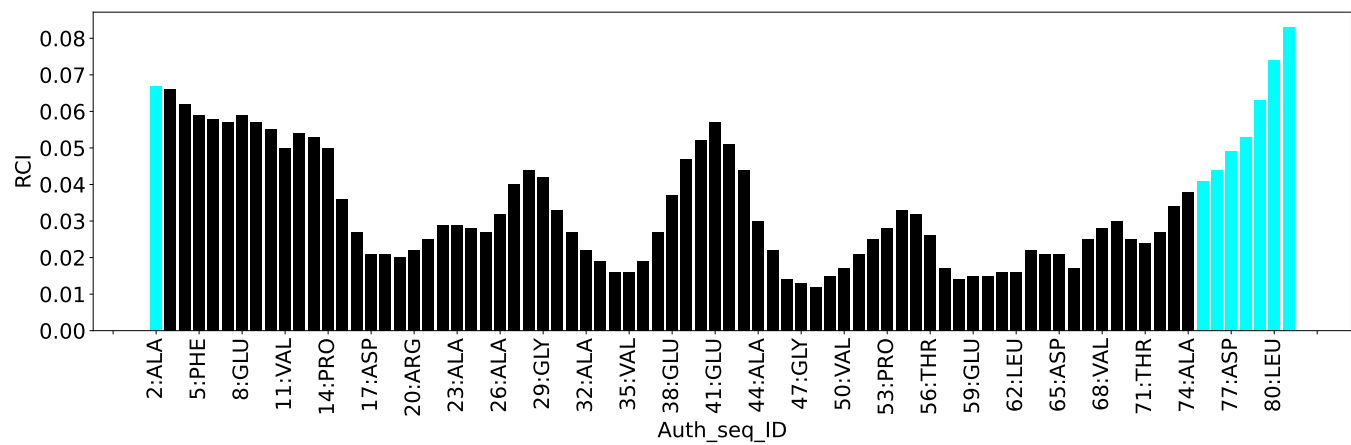
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	66	PHE	CD2	118.13	125.53 – 137.61	-11.1
1	A	66	PHE	CD1	118.13	125.33 – 137.83	-10.8
1	A	66	PHE	CZ	118.08	121.82 – 136.66	-7.5
1	A	61	HIS	CE1	123.91	126.08 – 149.12	-5.9
1	A	5	PHE	CE2	137.13	124.80 – 136.72	5.3
1	A	66	PHE	CE2	137.13	124.80 – 136.72	5.3
1	A	5	PHE	CZ	136.94	121.82 – 136.66	5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1045
Intra-residue ($ i-j =0$)	225
Sequential ($ i-j =1$)	288
Medium range ($ i-j >1$ and $ i-j <5$)	179
Long range ($ i-j \geq 5$)	347
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	0
Total dihedral-angle restraints	124
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue ¹	4.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	24.2	0.2
0.2-0.5 (Medium)	52.8	0.5
>0.5 (Large)	133.5	5.22

8.2.2 Average number of dihedral-angle violations per model [i](#)

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	7.3	4.83
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

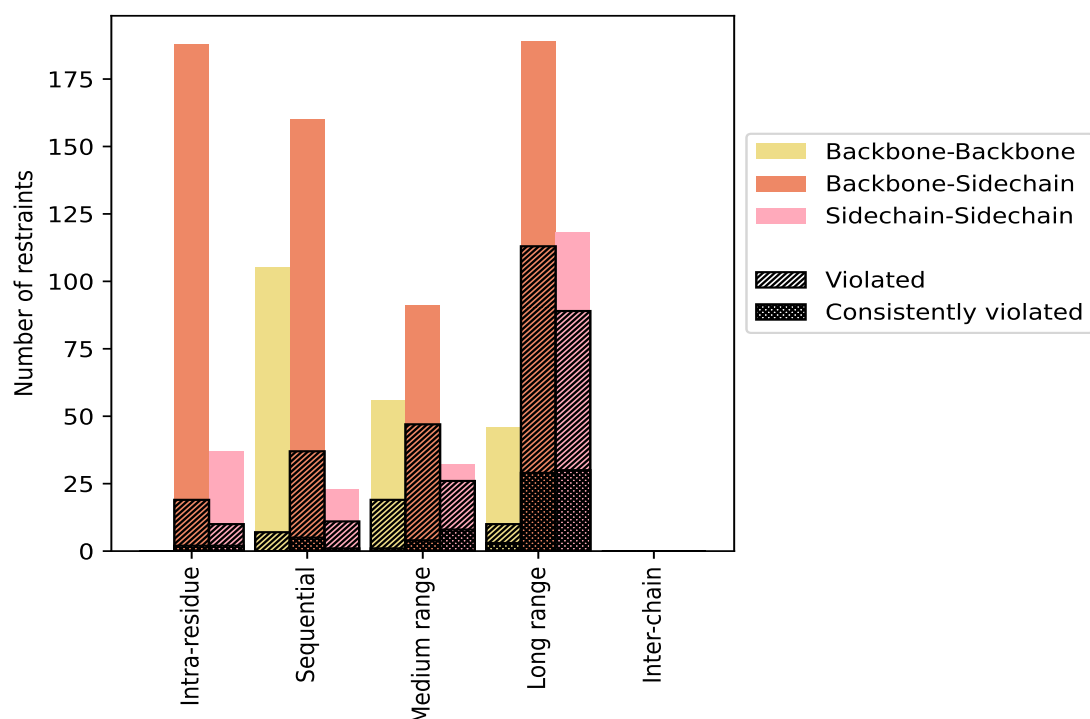
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	225	21.5	29	12.9	2.8	4	1.8	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	188	18.0	19	10.1	1.8	2	1.1	0.2
Sidechain-Sidechain	37	3.5	10	27.0	1.0	2	5.4	0.2
Sequential (i-j =1)	288	27.6	55	19.1	5.3	6	2.1	0.6
Backbone-Backbone	105	10.0	7	6.7	0.7	0	0.0	0.0
Backbone-Sidechain	160	15.3	37	23.1	3.5	5	3.1	0.5
Sidechain-Sidechain	23	2.2	11	47.8	1.1	1	4.3	0.1
Medium range (i-j >1 & i-j <5)	179	17.1	92	51.4	8.8	13	7.3	1.2
Backbone-Backbone	56	5.4	19	33.9	1.8	1	1.8	0.1
Backbone-Sidechain	91	8.7	47	51.6	4.5	4	4.4	0.4
Sidechain-Sidechain	32	3.1	26	81.2	2.5	8	25.0	0.8
Long range (i-j ≥5)	347	33.2	207	59.7	19.8	60	17.3	5.7
Backbone-Backbone	46	4.4	10	21.7	1.0	3	6.5	0.3
Backbone-Sidechain	183	17.5	108	59.0	10.3	27	14.8	2.6
Sidechain-Sidechain	118	11.3	89	75.4	8.5	30	25.4	2.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	0.6	5	83.3	0.5	2	33.3	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1045	100.0	388	37.1	37.1	85	8.1	8.1
Backbone-Backbone	207	19.8	36	17.4	3.4	4	1.9	0.4
Backbone-Sidechain	628	60.1	216	34.4	20.7	40	6.4	3.8
Sidechain-Sidechain	210	20.1	136	64.8	13.0	41	19.5	3.9

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

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



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

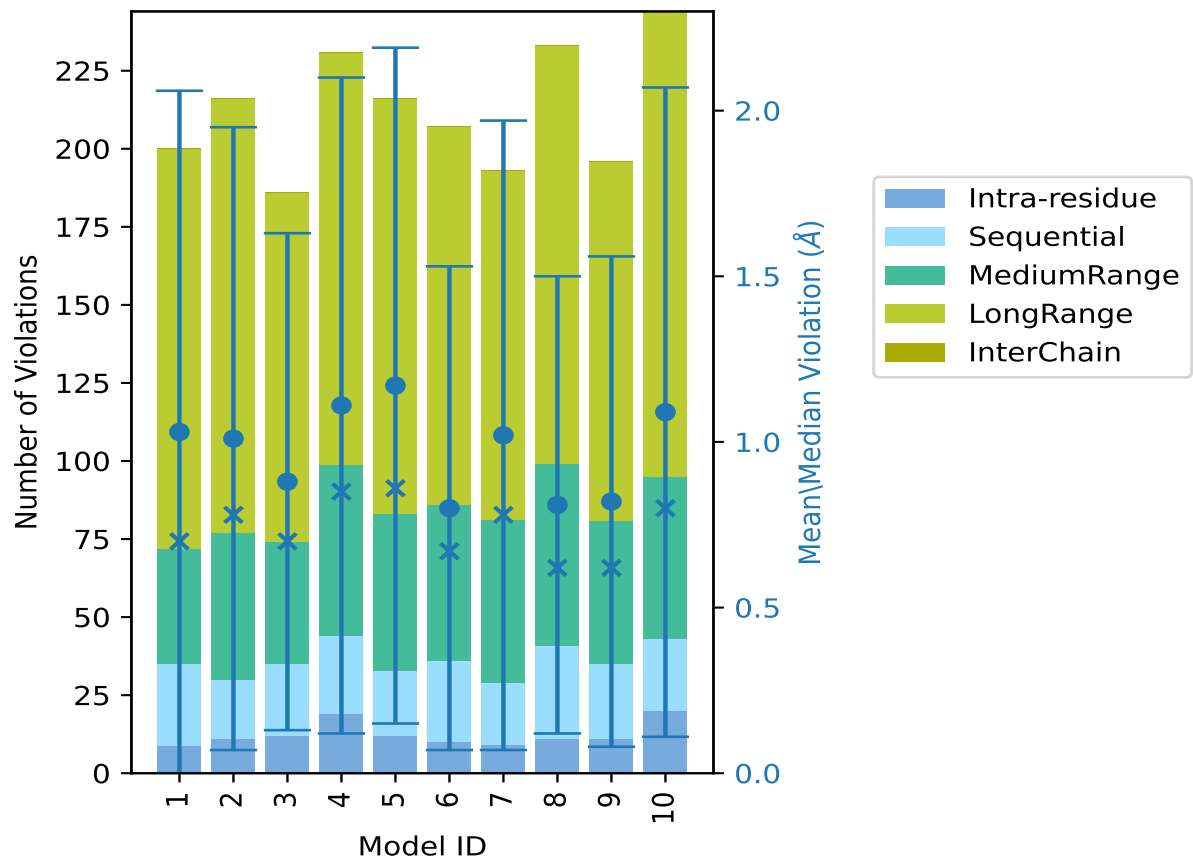
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	9	26	37	128	0	200	1.03	4.96	1.03	0.7
2	11	19	47	139	0	216	1.01	5.22	0.94	0.78
3	12	23	39	112	0	186	0.88	4.75	0.75	0.7
4	19	25	55	132	0	231	1.11	4.83	0.99	0.85
5	12	21	50	133	0	216	1.17	4.96	1.02	0.86
6	10	26	50	121	0	207	0.8	4.71	0.73	0.67
7	9	20	52	112	0	193	1.02	4.8	0.95	0.78
8	11	30	58	134	0	233	0.81	4.53	0.69	0.62
9	11	24	46	115	0	196	0.82	4.37	0.74	0.62
10	20	23	52	149	0	244	1.09	4.77	0.98	0.8

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 656(IR:196, SQ:233, MR:87, LR:140, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	14	14	24	0	57	1	10.0
4	3	11	19	0	37	2	20.0
7	9	3	16	0	35	3	30.0

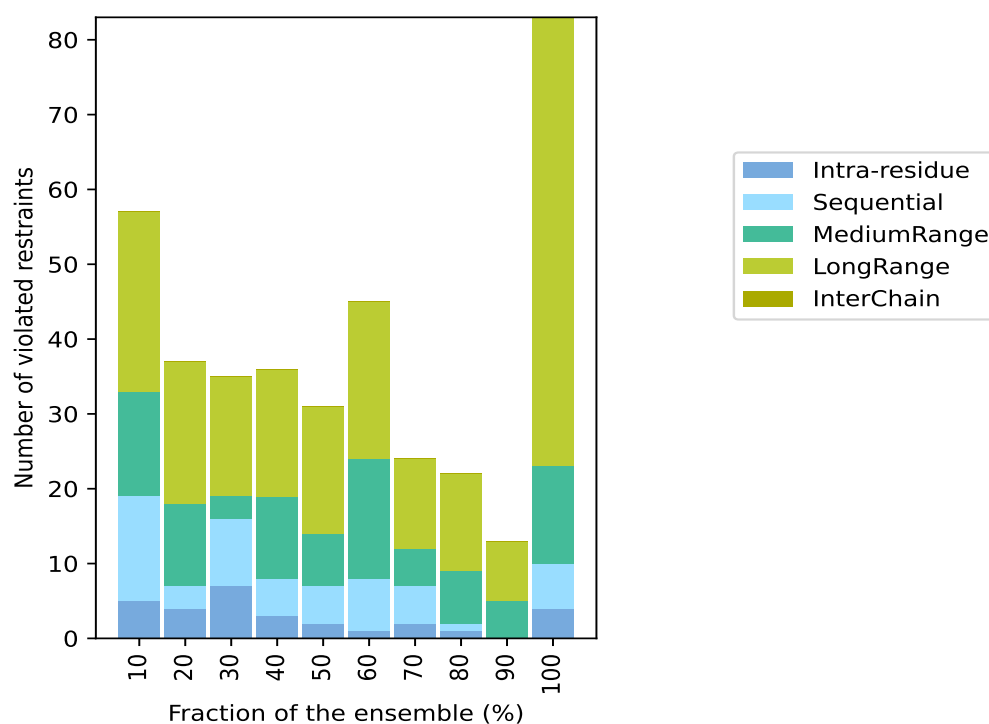
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	5	11	17	0	36	4	40.0
2	5	7	17	0	31	5	50.0
1	7	16	21	0	45	6	60.0
2	5	5	12	0	24	7	70.0
1	1	7	13	0	22	8	80.0
0	0	5	8	0	13	9	90.0
4	6	13	60	0	83	10	100.0

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

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

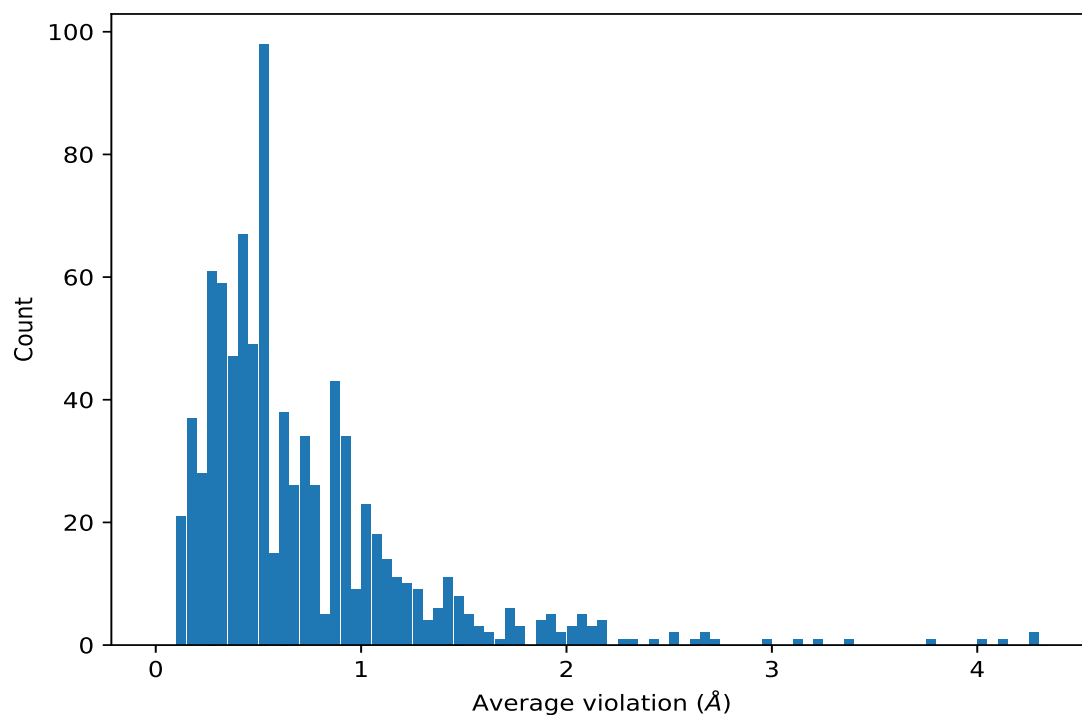


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	10	4.29	0.64	4.61
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	10	4.29	0.64	4.61
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	10	4.1	0.63	4.11
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	10	4.03	0.58	4.08
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	10	3.76	0.36	3.81
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	10	3.35	1.74	4.68
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	10	3.24	1.02	3.92
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	10	2.99	0.33	2.97
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	10	2.72	1.52	3.69
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	10	2.68	1.6	3.8
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	10	2.6	0.69	2.8
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	10	2.5	0.64	2.64
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	10	2.5	0.64	2.64
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	10	2.43	1.51	3.26
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	10	2.33	1.03	2.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	10	2.19	0.42	2.16
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	10	2.1	0.37	1.96
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	10	2.1	0.37	1.96
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	10	2.1	0.37	1.96
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	10	2.07	1.4	1.72
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	10	2.07	1.4	1.72
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	10	2.05	0.45	2.26
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	10	2.05	0.45	2.26
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	10	2.05	0.45	2.26
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	10	2.01	0.63	2.3
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	10	2.01	0.61	2.15
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	10	2.01	0.61	2.15
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	10	1.95	0.24	2.06
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	10	1.93	0.35	2.01
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	10	1.93	0.35	2.01
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	10	1.93	0.35	2.01
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	10	1.92	0.99	2.07
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	10	1.85	0.44	2.08
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	10	1.85	0.44	2.08
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	10	1.85	0.44	2.08
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	10	1.74	0.41	1.84
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	10	1.74	0.41	1.84
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	10	1.74	0.41	1.84
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	10	1.74	0.41	1.84
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	10	1.65	0.97	1.81
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	10	1.56	0.46	1.72
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	10	1.56	0.84	1.44
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	10	1.56	0.84	1.44
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	10	1.49	0.54	1.44
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	10	1.47	0.59	1.32
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	10	1.44	0.41	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	10	1.44	0.41	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	10	1.44	0.41	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	10	1.44	0.41	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	10	1.44	0.41	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	10	1.44	0.41	1.54
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	10	1.38	0.23	1.38
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	10	1.35	0.3	1.27
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	10	1.34	1.03	0.91
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	10	1.29	0.5	1.42
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	10	1.29	0.5	1.42
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	10	1.29	0.5	1.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	10	1.29	0.5	1.42
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	10	1.29	0.5	1.42
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	10	1.29	0.5	1.42
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	10	1.22	0.36	1.23
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	10	1.21	0.64	1.04
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	10	1.21	0.64	1.04
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	10	1.2	0.46	1.11
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	10	1.2	0.46	1.11
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	10	1.2	0.46	1.11
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	10	1.19	0.45	1.17
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	10	1.19	0.45	1.17
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	10	1.19	0.45	1.17
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	10	1.16	0.65	0.98
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	10	1.16	0.65	0.98
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	10	1.14	0.46	1.11
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	10	1.14	0.56	1.02
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	10	1.14	0.56	1.02
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	10	1.13	0.29	1.15
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	10	1.12	0.39	1.16
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	10	1.09	0.72	0.85
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	10	1.08	0.24	1.01
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	10	1.08	0.39	1.16
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	10	1.08	0.39	1.16
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	10	1.08	0.39	1.16
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	10	1.06	0.04	1.06
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	10	1.05	0.03	1.05
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	10	1.05	0.03	1.05
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	10	1.05	0.03	1.05
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	10	1.05	0.19	1.09
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	10	1.03	0.75	0.86
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	10	1.03	0.33	0.98
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	10	1.03	0.33	0.98
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	10	1.03	0.33	0.98
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	10	1.03	0.31	1.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	10	1.03	0.31	1.02
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	10	1.03	0.31	1.02
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	10	1.02	0.05	1.02
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	10	0.96	0.25	0.95
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	10	0.94	0.28	0.92
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	10	0.94	0.28	0.92
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	10	0.93	0.3	1.02
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	10	0.93	0.3	1.02
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	10	0.93	0.3	1.02
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	10	0.93	0.3	1.02
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	10	0.93	0.3	1.02
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	10	0.93	0.3	1.02
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	10	0.93	0.2	0.88
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	10	0.93	0.23	0.96
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	10	0.92	0.14	0.94
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	10	0.89	0.31	0.88
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	10	0.89	0.31	0.88
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	10	0.89	0.31	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	10	0.89	0.31	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	10	0.89	0.31	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	10	0.89	0.31	0.88
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	10	0.89	0.41	0.84
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	10	0.88	0.41	0.88
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	10	0.88	0.41	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	10	0.88	0.05	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	10	0.88	0.05	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	10	0.88	0.05	0.88
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	10	0.88	0.35	0.97
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	10	0.88	0.35	0.97
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	10	0.88	0.35	0.97
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	10	0.87	0.19	0.76
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	10	0.84	0.29	0.78
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	10	0.84	0.2	0.9
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	10	0.79	0.21	0.8
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	10	0.76	0.28	0.74
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	10	0.76	0.28	0.74
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	10	0.76	0.28	0.74
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	10	0.75	0.23	0.7
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	10	0.74	0.41	0.8
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	10	0.73	0.25	0.67
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	10	0.7	0.03	0.7
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	10	0.7	0.19	0.7
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	10	0.7	0.22	0.7
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	10	0.68	0.29	0.82
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	10	0.66	0.21	0.66
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	10	0.64	0.23	0.66
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	10	0.63	0.13	0.6
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	10	0.62	0.19	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	10	0.6	0.01	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	10	0.6	0.01	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	10	0.6	0.01	0.6
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	10	0.54	0.14	0.46
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	10	0.52	0.25	0.5
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	10	0.49	0.09	0.48
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	10	0.27	0.04	0.27
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	9	1.6	0.13	1.67
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	9	1.36	1.09	0.81
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	9	1.12	0.97	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	9	1.0	0.39	0.92
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	9	1.0	0.39	0.92
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	9	0.91	0.6	0.69
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	9	0.91	0.6	0.69
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	9	0.87	0.38	0.93
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	9	0.8	0.33	0.82
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	9	0.8	0.33	0.82
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	9	0.71	0.51	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	9	0.71	0.51	0.49
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	9	0.44	0.19	0.4
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	9	0.43	0.24	0.35
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	9	0.38	0.45	0.22
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	9	0.38	0.45	0.22
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	9	0.38	0.45	0.22
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	9	0.37	0.17	0.35
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	9	0.32	0.14	0.35
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	8	1.73	1.7	0.62
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	8	1.73	1.7	0.62
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	8	1.48	0.83	1.41
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	8	1.48	0.83	1.41
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	8	1.48	0.83	1.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	8	1.41	0.3	1.52
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	8	1.32	0.56	1.2
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	8	1.32	0.56	1.2
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	8	1.32	0.56	1.2
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	8	1.2	0.7	1.2
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	8	1.2	0.7	1.2
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	8	1.17	0.27	1.1
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	8	1.04	0.51	1.0
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	8	0.92	0.52	0.97
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	8	0.91	0.34	1.07
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	8	0.91	0.34	1.07
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	8	0.88	0.3	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	8	0.88	0.3	0.97
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	8	0.82	0.15	0.8
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	8	0.77	0.43	0.84
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	8	0.76	0.29	0.8
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	8	0.55	0.24	0.46
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	8	0.54	0.22	0.5
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	8	0.54	0.22	0.5
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	8	0.54	0.22	0.5
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	8	0.54	0.33	0.47
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	8	0.54	0.34	0.57
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	8	0.53	0.2	0.61
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	8	0.53	0.2	0.61
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	8	0.53	0.2	0.61
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	8	0.43	0.18	0.46
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	8	0.33	0.13	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	8	0.33	0.19	0.26
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	8	0.14	0.03	0.13
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	7	1.97	0.75	2.19
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	7	1.46	0.24	1.37
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	7	0.93	0.27	1.07
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	7	0.9	0.14	0.86
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	7	0.9	0.14	0.86
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	7	0.75	0.26	0.65
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	7	0.75	0.26	0.65
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	7	0.71	0.16	0.65
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	7	0.68	0.32	0.85
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	7	0.68	0.32	0.85
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	7	0.68	0.32	0.85
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	7	0.68	0.32	0.85
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	7	0.68	0.32	0.85
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	7	0.68	0.32	0.85
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	7	0.64	0.38	0.47
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	7	0.64	0.38	0.47
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	7	0.64	0.38	0.47
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	7	0.63	0.36	0.59
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	7	0.63	0.36	0.59
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	7	0.51	0.21	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	7	0.51	0.21	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	7	0.51	0.21	0.41
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	7	0.5	0.15	0.42
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	7	0.49	0.33	0.42
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	7	0.46	0.23	0.59
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	7	0.44	0.2	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	7	0.44	0.2	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	7	0.44	0.2	0.4
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	7	0.41	0.2	0.41
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	7	0.36	0.21	0.42
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	7	0.35	0.19	0.37
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	7	0.3	0.15	0.27
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	7	0.29	0.1	0.28
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	7	0.27	0.07	0.28
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	7	0.27	0.08	0.25
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	7	0.23	0.09	0.23
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	7	0.23	0.09	0.23
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	7	0.23	0.09	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	7	0.21	0.06	0.23
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	7	0.12	0.01	0.12
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	7	0.12	0.01	0.12
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	7	0.12	0.01	0.12
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	6	2.17	0.23	2.22
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	6	1.91	0.09	1.92
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	6	1.89	0.81	1.82
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	6	1.76	0.21	1.76
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	6	1.76	0.21	1.76
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	6	1.76	0.21	1.76
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	6	1.54	0.45	1.79
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	6	1.54	0.45	1.79
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	6	1.54	0.45	1.79
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	6	1.47	0.25	1.53
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	6	1.46	0.68	1.65
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	6	1.4	0.52	1.5
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	6	1.37	0.45	1.39
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	6	1.37	0.45	1.39
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	6	1.37	0.45	1.39
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	6	1.29	0.91	1.39
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	6	1.29	0.91	1.39
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	6	1.12	0.56	1.24
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	6	1.12	0.56	1.24
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	6	1.11	0.54	1.07
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	6	1.11	0.54	1.07
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	6	1.11	0.54	1.07
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	6	0.99	0.55	0.97
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	6	0.99	0.55	0.97
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	6	0.99	0.55	0.97
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	6	0.99	0.55	0.97
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	6	0.99	0.55	0.97
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	6	0.99	0.55	0.97
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	6	0.91	0.28	1.0
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	6	0.91	0.28	1.0
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	6	0.76	0.24	0.85
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	6	0.73	0.54	0.52
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	6	0.73	0.54	0.52
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	6	0.73	0.54	0.52
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	6	0.71	0.57	0.7
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	6	0.68	0.34	0.54
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	6	0.68	0.34	0.54
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	6	0.68	0.34	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	6	0.68	0.27	0.7
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	6	0.68	0.27	0.7
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	6	0.68	0.27	0.7
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	6	0.67	0.37	0.69
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	6	0.67	0.37	0.69
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	6	0.63	0.38	0.46
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	6	0.63	0.38	0.46
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	6	0.63	0.38	0.46
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	6	0.58	0.32	0.54
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	6	0.56	0.33	0.59
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	6	0.56	0.33	0.59
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	6	0.56	0.33	0.59
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	6	0.56	0.33	0.59
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	6	0.56	0.33	0.59
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	6	0.56	0.33	0.59
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	6	0.52	0.35	0.4
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	6	0.5	0.26	0.49
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	6	0.5	0.26	0.49
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	6	0.5	0.37	0.38
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	6	0.5	0.37	0.38
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	6	0.47	0.2	0.42
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	6	0.47	0.2	0.42
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	6	0.47	0.2	0.42
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	6	0.47	0.2	0.42
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	6	0.47	0.2	0.42
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	6	0.47	0.2	0.42
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	6	0.46	0.19	0.42
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	6	0.46	0.36	0.32
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	6	0.46	0.36	0.32
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	6	0.43	0.22	0.36
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	6	0.42	0.16	0.38
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	6	0.39	0.3	0.26
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	6	0.39	0.3	0.26
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	6	0.39	0.3	0.26
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	6	0.38	0.26	0.29
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	6	0.38	0.26	0.29
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	6	0.38	0.26	0.29
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	6	0.32	0.19	0.25
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	6	0.32	0.19	0.25
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	6	0.32	0.19	0.25
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	6	0.32	0.1	0.34
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	6	0.3	0.13	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	6	0.3	0.09	0.3
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	6	0.3	0.09	0.3
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	6	0.3	0.09	0.3
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	6	0.3	0.06	0.31
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	6	0.3	0.06	0.31
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	6	0.3	0.06	0.31
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	6	0.3	0.15	0.25
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	6	0.3	0.15	0.25
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	6	0.27	0.08	0.26
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	6	0.27	0.08	0.26
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	6	0.26	0.07	0.26
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	6	0.23	0.08	0.22
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	6	0.19	0.06	0.2
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	6	0.17	0.04	0.16
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	6	0.17	0.04	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	6	0.15	0.03	0.15
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	6	0.15	0.03	0.15
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	6	0.15	0.03	0.15
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	6	0.15	0.03	0.15
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	6	0.15	0.03	0.15
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	6	0.15	0.03	0.15
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	5	2.25	1.55	2.95
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	5	2.15	1.18	2.53
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	5	1.4	0.35	1.37
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	5	1.27	1.01	1.55
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	5	1.18	0.73	0.96
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	5	1.18	0.73	0.96
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	5	1.18	0.73	0.96
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	5	1.06	0.21	1.12
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	5	1.06	0.21	1.12
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	5	1.06	0.21	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	5	1.06	0.21	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	5	1.06	0.21	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	5	1.06	0.21	1.12
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	5	0.94	0.08	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	5	0.92	0.35	0.84
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	5	0.92	0.35	0.84
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	5	0.85	0.45	1.0
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	5	0.85	0.45	1.0
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	5	0.85	0.45	1.0
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	5	0.76	0.49	0.51
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	5	0.72	0.18	0.67
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	5	0.52	0.03	0.5
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	5	0.47	0.18	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	5	0.47	0.18	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	5	0.47	0.18	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	5	0.47	0.18	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	5	0.47	0.18	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	5	0.47	0.18	0.41
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	5	0.46	0.18	0.52
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	5	0.46	0.18	0.52
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	5	0.45	0.19	0.51
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	5	0.43	0.15	0.47
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	5	0.4	0.34	0.21
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	5	0.4	0.34	0.21
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	5	0.4	0.34	0.21
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	5	0.38	0.15	0.41
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	5	0.36	0.19	0.45
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	5	0.36	0.19	0.45
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	5	0.36	0.19	0.45
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	5	0.33	0.14	0.29
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	5	0.32	0.25	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	5	0.32	0.25	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	5	0.32	0.25	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	5	0.32	0.25	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	5	0.32	0.25	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	5	0.32	0.25	0.22
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	5	0.3	0.11	0.35
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	5	0.3	0.12	0.29
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	5	0.3	0.12	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	5	0.3	0.12	0.29
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	5	0.3	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	5	0.3	0.12	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	5	0.3	0.12	0.29
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	5	0.29	0.09	0.3
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	5	0.29	0.09	0.3
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	5	0.29	0.09	0.3
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	5	0.28	0.16	0.24
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	5	0.28	0.16	0.24
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	5	0.28	0.06	0.26
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	5	0.27	0.11	0.22
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	5	0.27	0.11	0.22
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	5	0.26	0.09	0.23
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	5	0.26	0.09	0.23
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	5	0.26	0.09	0.23
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	5	0.23	0.09	0.23
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	5	0.2	0.05	0.19
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	5	0.18	0.11	0.11
(1,607)	1:46:A:TYR:HD2	1:64:A:ARG:HA	4	2.18	1.2	2.58
(1,482)	1:37:A:THR:HA	1:46:A:TYR:HD1	4	1.64	0.87	1.94
(1,142)	1:15:A:ASP:HB2	1:18:A:ARG:HB2	4	1.23	0.61	1.48
(1,142)	1:15:A:ASP:HB3	1:18:A:ARG:HB2	4	1.23	0.61	1.48
(1,483)	1:37:A:THR:HA	1:46:A:TYR:HE1	4	1.16	0.56	1.29
(1,123)	1:15:A:ASP:H	1:18:A:ARG:HG2	4	1.15	0.24	1.14
(1,149)	1:15:A:ASP:HB2	1:66:A:PHE:HZ	4	1.01	0.55	0.87
(1,149)	1:15:A:ASP:HB3	1:66:A:PHE:HZ	4	1.01	0.55	0.87
(1,202)	1:18:A:ARG:HB2	1:66:A:PHE:HE1	4	0.93	0.56	0.7
(1,919)	1:63:A:ASP:HB2	1:64:A:ARG:HG3	4	0.91	0.14	0.92
(1,556)	1:44:A:ALA:HB1	1:61:A:HIS:HD2	4	0.91	0.4	1.02
(1,556)	1:44:A:ALA:HB2	1:61:A:HIS:HD2	4	0.91	0.4	1.02
(1,556)	1:44:A:ALA:HB3	1:61:A:HIS:HD2	4	0.91	0.4	1.02
(1,811)	1:59:A:GLU:HG3	1:74:A:ALA:HA	4	0.86	0.24	0.98
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD2	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD2	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD2	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD2	4	0.77	0.35	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD2	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD2	4	0.77	0.35	0.78
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD3	4	0.77	0.35	0.78
(1,954)	1:65:A:ASP:HB2	1:67:A:ARG:HA	4	0.68	0.36	0.71
(1,117)	1:14:A:PRO:HG2	1:16:A:ALA:H	4	0.66	0.64	0.3
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG11	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG12	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG13	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG21	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG22	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG23	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG11	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG12	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG13	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG21	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG22	4	0.64	0.3	0.65
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG23	4	0.64	0.3	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG11	4	0.64	0.27	0.68
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG12	4	0.64	0.27	0.68
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG13	4	0.64	0.27	0.68
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG21	4	0.64	0.27	0.68
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG22	4	0.64	0.27	0.68
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG23	4	0.64	0.27	0.68
(1,974)	1:67:A:ARG:HG2	1:68:A:VAL:HB	4	0.62	0.31	0.54
(1,974)	1:67:A:ARG:HG3	1:68:A:VAL:HB	4	0.62	0.31	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG11	4	0.53	0.24	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG12	4	0.53	0.24	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG13	4	0.53	0.24	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG21	4	0.53	0.24	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG22	4	0.53	0.24	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG23	4	0.53	0.24	0.54
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB2	4	0.5	0.14	0.46
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB3	4	0.5	0.14	0.46
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB1	4	0.45	0.25	0.44
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB2	4	0.45	0.25	0.44
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB3	4	0.45	0.25	0.44
(1,311)	1:23:A:ALA:HB1	1:51:A:THR:H	4	0.43	0.18	0.38
(1,311)	1:23:A:ALA:HB2	1:51:A:THR:H	4	0.43	0.18	0.38
(1,311)	1:23:A:ALA:HB3	1:51:A:THR:H	4	0.43	0.18	0.38
(1,721)	1:52:A:ARG:HG2	1:56:A:THR:H	4	0.43	0.13	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB1	4	0.39	0.24	0.36
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB2	4	0.39	0.24	0.36
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB3	4	0.39	0.24	0.36
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD2	4	0.38	0.16	0.39
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD3	4	0.38	0.16	0.39
(1,160)	1:16:A:ALA:HA	1:19:A:ALA:H	4	0.35	0.14	0.36
(1,693)	1:51:A:THR:HG21	1:54:A:ASP:H	4	0.34	0.16	0.36
(1,693)	1:51:A:THR:HG22	1:54:A:ASP:H	4	0.34	0.16	0.36
(1,693)	1:51:A:THR:HG23	1:54:A:ASP:H	4	0.34	0.16	0.36
(1,87)	1:10:A:GLU:HA	1:11:A:VAL:H	4	0.34	0.08	0.3
(1,209)	1:18:A:ARG:HG2	1:20:A:ARG:H	4	0.32	0.22	0.28
(1,96)	1:11:A:VAL:HB	1:12:A:THR:H	4	0.32	0.02	0.31
(1,248)	1:20:A:ARG:HB2	1:35:A:VAL:H	4	0.31	0.09	0.3
(1,771)	1:57:A:ARG:HB2	1:74:A:ALA:H	4	0.3	0.14	0.26
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	4	0.28	0.15	0.26
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	4	0.28	0.15	0.26
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	4	0.28	0.15	0.26
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	4	0.28	0.15	0.26
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	4	0.28	0.15	0.26
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	4	0.28	0.15	0.26
(1,263)	1:20:A:ARG:HG3	1:34:A:GLU:H	4	0.27	0.07	0.29
(1,937)	1:64:A:ARG:HA	1:64:A:ARG:HG2	4	0.26	0.08	0.26
(1,584)	1:46:A:TYR:HA	1:62:A:LEU:HB3	4	0.23	0.14	0.17
(1,946)	1:64:A:ARG:HG2	1:66:A:PHE:H	4	0.18	0.07	0.15
(1,946)	1:64:A:ARG:HG3	1:66:A:PHE:H	4	0.18	0.07	0.15
(1,663)	1:50:A:VAL:H	1:50:A:VAL:HB	4	0.14	0.04	0.12
(1,610)	1:46:A:TYR:HE2	1:64:A:ARG:HA	3	3.1	0.57	2.76
(1,608)	1:46:A:TYR:HD2	1:66:A:PHE:H	3	2.66	0.01	2.66
(1,140)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	3	1.54	0.42	1.75
(1,137)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	3	1.51	0.54	1.17
(1,147)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	3	1.43	0.04	1.42
(1,147)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	3	1.43	0.04	1.42
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG21	3	1.14	0.59	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG22	3	1.14	0.59	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG23	3	1.14	0.59	1.56
(1,585)	1:46:A:TYR:HB2	1:46:A:TYR:HD2	3	1.08	0.02	1.08
(1,604)	1:46:A:TYR:HD1	1:47:A:GLY:H	3	1.06	0.04	1.04
(1,581)	1:46:A:TYR:HA	1:46:A:TYR:HD1	3	1.02	0.15	0.93
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB1	3	0.67	0.26	0.82
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB2	3	0.67	0.26	0.82
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB3	3	0.67	0.26	0.82
(1,573)	1:46:A:TYR:H	1:46:A:TYR:HD2	3	0.62	0.12	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	3	0.57	0.01	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	3	0.57	0.01	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	3	0.57	0.01	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	3	0.57	0.01	0.57
(1,473)	1:36:A:GLU:HG3	1:47:A:GLY:H	3	0.54	0.33	0.61
(1,387)	1:27:A:VAL:HG11	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,387)	1:27:A:VAL:HG12	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,387)	1:27:A:VAL:HG13	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,387)	1:27:A:VAL:HG21	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,387)	1:27:A:VAL:HG22	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,387)	1:27:A:VAL:HG23	1:50:A:VAL:HB	3	0.53	0.09	0.53
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	3	0.52	0.25	0.45
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	3	0.52	0.25	0.45
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	3	0.52	0.25	0.45
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB2	3	0.52	0.23	0.56
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB2	3	0.52	0.23	0.56
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB2	3	0.52	0.23	0.56
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB3	3	0.52	0.23	0.56
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB3	3	0.52	0.23	0.56
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB3	3	0.52	0.23	0.56
(1,595)	1:46:A:TYR:HB3	1:46:A:TYR:HE1	3	0.52	0.01	0.52
(1,61)	1:6:A:ASP:H	1:7:A:GLY:H	3	0.5	0.15	0.44
(1,557)	1:44:A:ALA:HB1	1:62:A:LEU:H	3	0.49	0.16	0.45
(1,557)	1:44:A:ALA:HB2	1:62:A:LEU:H	3	0.49	0.16	0.45
(1,557)	1:44:A:ALA:HB3	1:62:A:LEU:H	3	0.49	0.16	0.45
(1,802)	1:59:A:GLU:H	1:74:A:ALA:HA	3	0.46	0.18	0.38
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG11	3	0.43	0.18	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG12	3	0.43	0.18	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG13	3	0.43	0.18	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG21	3	0.43	0.18	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG22	3	0.43	0.18	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG23	3	0.43	0.18	0.44
(1,371)	1:27:A:VAL:HA	1:28:A:PRO:HB3	3	0.37	0.1	0.43
(1,920)	1:63:A:ASP:HB2	1:65:A:ASP:H	3	0.36	0.13	0.42
(1,591)	1:46:A:TYR:HB2	1:66:A:PHE:HA	3	0.34	0.07	0.33
(1,506)	1:38:A:GLU:HB2	1:40:A:GLY:H	3	0.34	0.21	0.27
(1,506)	1:38:A:GLU:HB3	1:40:A:GLY:H	3	0.34	0.21	0.27
(1,814)	1:59:A:GLU:HG2	1:74:A:ALA:HA	3	0.34	0.13	0.36
(1,814)	1:59:A:GLU:HG3	1:74:A:ALA:HA	3	0.34	0.13	0.36
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB1	3	0.25	0.15	0.16
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB2	3	0.25	0.15	0.16
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB3	3	0.25	0.15	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4)	1:31:A:THR:O	1:51:A:THR:H	3	0.25	0.1	0.26
(1,516)	1:39:A:THR:HA	1:39:A:THR:HB	3	0.24	0.0	0.24
(1,655)	1:49:A:LEU:HB3	1:49:A:LEU:HG	3	0.22	0.08	0.27
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB1	3	0.19	0.06	0.2
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB2	3	0.19	0.06	0.2
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB3	3	0.19	0.06	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB1	3	0.19	0.06	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB2	3	0.19	0.06	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB3	3	0.19	0.06	0.2
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB2	3	0.19	0.07	0.23
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB3	3	0.19	0.07	0.23
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD2	3	0.19	0.03	0.18
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD3	3	0.19	0.03	0.18
(1,653)	1:49:A:LEU:HB2	1:50:A:VAL:H	3	0.17	0.05	0.14
(1,1032)	1:79:A:GLY:H	1:80:A:LEU:H	3	0.16	0.03	0.17
(1,950)	1:65:A:ASP:HA	1:66:A:PHE:HB3	3	0.14	0.0	0.14
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD2	2	0.98	0.28	0.98
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD3	2	0.98	0.28	0.98
(1,513)	1:38:A:GLU:HG2	1:46:A:TYR:HA	2	0.75	0.36	0.75
(1,513)	1:38:A:GLU:HG3	1:46:A:TYR:HA	2	0.75	0.36	0.75
(1,217)	1:19:A:ALA:H	1:66:A:PHE:HE1	2	0.75	0.34	0.75
(1,146)	1:15:A:ASP:HB2	1:37:A:THR:H	2	0.68	0.2	0.68
(1,146)	1:15:A:ASP:HB3	1:37:A:THR:H	2	0.68	0.2	0.68
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB1	2	0.66	0.36	0.66
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB2	2	0.66	0.36	0.66
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB3	2	0.66	0.36	0.66
(1,535)	1:43:A:ALA:HB1	1:63:A:ASP:HB2	2	0.6	0.2	0.6
(1,535)	1:43:A:ALA:HB2	1:63:A:ASP:HB2	2	0.6	0.2	0.6
(1,535)	1:43:A:ALA:HB3	1:63:A:ASP:HB2	2	0.6	0.2	0.6
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB1	2	0.56	0.12	0.56
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB2	2	0.56	0.12	0.56
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB3	2	0.56	0.12	0.56
(1,101)	1:12:A:THR:HA	1:12:A:THR:HB	2	0.52	0.01	0.52
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD23	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD23	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD23	2	0.5	0.29	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD23	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD23	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD21	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD22	2	0.5	0.29	0.5
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD23	2	0.5	0.29	0.5
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB2	2	0.45	0.32	0.45
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB2	2	0.45	0.32	0.45
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB2	2	0.45	0.32	0.45
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB3	2	0.45	0.32	0.45
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB3	2	0.45	0.32	0.45
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB3	2	0.45	0.32	0.45
(1,135)	1:15:A:ASP:HB2	1:18:A:ARG:H	2	0.44	0.29	0.44
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG11	2	0.39	0.18	0.39
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG12	2	0.39	0.18	0.39
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG13	2	0.39	0.18	0.39
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG21	2	0.39	0.18	0.39
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG22	2	0.39	0.18	0.39
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG23	2	0.39	0.18	0.39
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG2	2	0.38	0.21	0.38
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG3	2	0.38	0.21	0.38
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG11	2	0.37	0.1	0.37
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG12	2	0.37	0.1	0.37
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG13	2	0.37	0.1	0.37
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG21	2	0.37	0.1	0.37
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG22	2	0.37	0.1	0.37
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG23	2	0.37	0.1	0.37
(1,553)	1:44:A:ALA:HB1	1:46:A:TYR:H	2	0.36	0.09	0.36
(1,553)	1:44:A:ALA:HB2	1:46:A:TYR:H	2	0.36	0.09	0.36
(1,553)	1:44:A:ALA:HB3	1:46:A:TYR:H	2	0.36	0.09	0.36
(1,241)	1:20:A:ARG:HA	1:23:A:ALA:HA	2	0.35	0.07	0.35
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD21	2	0.3	0.18	0.3
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD22	2	0.3	0.18	0.3
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD23	2	0.3	0.18	0.3
(1,99)	1:12:A:THR:H	1:12:A:THR:HG21	2	0.29	0.01	0.29
(1,99)	1:12:A:THR:H	1:12:A:THR:HG22	2	0.29	0.01	0.29
(1,99)	1:12:A:THR:H	1:12:A:THR:HG23	2	0.29	0.01	0.29
(1,273)	1:21:A:ALA:H	1:24:A:VAL:H	2	0.29	0.1	0.29
(1,180)	1:17:A:ASP:HA	1:20:A:ARG:HB3	2	0.28	0.12	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,498)	1:38:A:GLU:H	1:46:A:TYR:HB3	2	0.28	0.09	0.28
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB2	2	0.27	0.01	0.27
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB3	2	0.27	0.01	0.27
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG11	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG12	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG13	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG21	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG22	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG23	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG11	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG12	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG13	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG21	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG22	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG23	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG11	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG12	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG13	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG21	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG22	2	0.26	0.08	0.26
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG23	2	0.26	0.08	0.26
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB2	2	0.22	0.12	0.22
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB2	2	0.22	0.12	0.22
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB2	2	0.22	0.12	0.22
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB3	2	0.22	0.12	0.22
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB3	2	0.22	0.12	0.22
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB3	2	0.22	0.12	0.22
(2,3)	1:31:A:THR:O	1:51:A:THR:N	2	0.21	0.04	0.21
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD2	2	0.2	0.04	0.2
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD3	2	0.2	0.04	0.2
(1,450)	1:35:A:VAL:HG11	1:47:A:GLY:H	2	0.2	0.03	0.2
(1,450)	1:35:A:VAL:HG12	1:47:A:GLY:H	2	0.2	0.03	0.2
(1,450)	1:35:A:VAL:HG13	1:47:A:GLY:H	2	0.2	0.03	0.2
(1,823)	1:60:A:VAL:HA	1:72:A:GLU:H	2	0.2	0.09	0.2
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG11	2	0.18	0.08	0.18
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG12	2	0.18	0.08	0.18
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG13	2	0.18	0.08	0.18
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG21	2	0.18	0.08	0.18
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG22	2	0.18	0.08	0.18
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG23	2	0.18	0.08	0.18
(1,984)	1:68:A:VAL:HA	1:70:A:ASP:H	2	0.18	0.06	0.18
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB1	2	0.17	0.06	0.17

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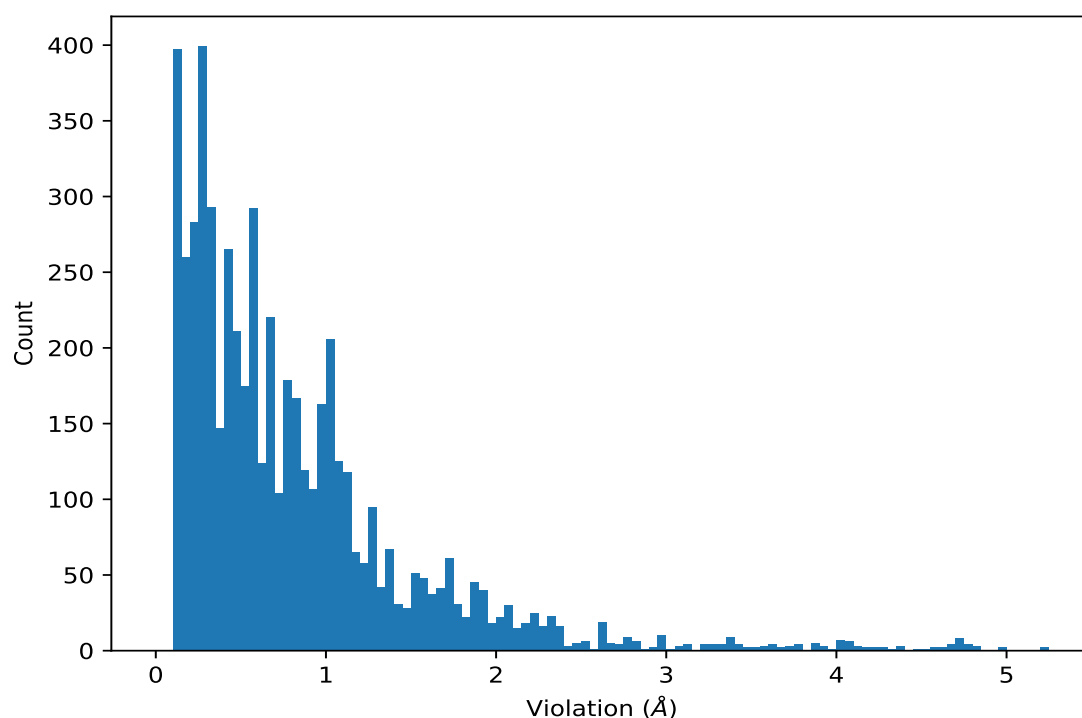
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB2	2	0.17	0.06	0.17
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB3	2	0.17	0.06	0.17
(1,543)	1:44:A:ALA:HA	1:46:A:TYR:H	2	0.17	0.02	0.17
(1,1018)	1:72:A:GLU:HB2	1:73:A:PRO:HA	2	0.16	0.05	0.16
(1,1018)	1:72:A:GLU:HB3	1:73:A:PRO:HA	2	0.16	0.05	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG11	2	0.14	0.02	0.14
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG12	2	0.14	0.02	0.14
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG13	2	0.14	0.02	0.14
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG21	2	0.14	0.02	0.14
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG22	2	0.14	0.02	0.14
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG23	2	0.14	0.02	0.14
(1,308)	1:23:A:ALA:HB1	1:48:A:VAL:HB	2	0.13	0.03	0.13
(1,308)	1:23:A:ALA:HB2	1:48:A:VAL:HB	2	0.13	0.03	0.13
(1,308)	1:23:A:ALA:HB3	1:48:A:VAL:HB	2	0.13	0.03	0.13
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB1	2	0.12	0.02	0.12
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB2	2	0.12	0.02	0.12
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB3	2	0.12	0.02	0.12
(1,580)	1:46:A:TYR:H	1:63:A:ASP:HA	2	0.11	0.0	0.11
(1,14)	1:3:A:MET:HB2	1:3:A:MET:HG3	2	0.1	0.0	0.1
(1,14)	1:3:A:MET:HB3	1:3:A:MET:HG3	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	2	5.22
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	2	5.22
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	5	4.96
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	1	4.96
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	4	4.83
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	4	4.83
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	2	4.82
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	7	4.8
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	1	4.78
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	10	4.77
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	3	4.75
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	5	4.73
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	5	4.73
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	2	4.71
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	2	4.71
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	6	4.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	6	4.71
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	2	4.7
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	7	4.7
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	1	4.68
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	4	4.68
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	7	4.67
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	7	4.67
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	5	4.62
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	5	4.62
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	3	4.6
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	3	4.6
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	8	4.53
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	10	4.46
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	1	4.37
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	1	4.37
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	9	4.37
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	1	4.3
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	10	4.28
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	3	4.28
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	4	4.21
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	1	4.21
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	4	4.15
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	5	4.15
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	6	4.13
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	4	4.12
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	1	4.12
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	3	4.09
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	9	4.09
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	9	4.09
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	5	4.08
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	5	4.06
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	4	4.05
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	10	4.04
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	10	4.03
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	10	4.03
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	1	4.03
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	7	4.03
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	10	4.01
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	7	4.0
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	4	3.96
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	2	3.93
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	9	3.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	5	3.91
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	1	3.9
(1,610)	1:46:A:TYR:HE2	1:64:A:ARG:HA	5	3.9
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	7	3.9
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	10	3.87
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	6	3.87
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	9	3.76
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	7	3.76
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	8	3.75
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	7	3.75
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	5	3.71
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	5	3.71
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	2	3.7
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	6	3.69
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	10	3.66
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	10	3.65
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	10	3.65
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	5	3.65
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	2	3.62
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	10	3.58
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	10	3.57
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	4	3.56
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	8	3.53
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	4	3.51
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	4	3.48
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	4	3.48
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	1	3.43
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	8	3.42
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	4	3.41
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	4	3.41
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	5	3.4
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	7	3.4
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	4	3.4
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	5	3.39
(1,607)	1:46:A:TYR:HD2	1:64:A:ARG:HA	5	3.37
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	2	3.37
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	4	3.37
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	10	3.36
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	10	3.36
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	2	3.34
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	2	3.34
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	1	3.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:A:MET:HA	1:5:A:PHE:HE1	5	3.32
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	4	3.3
(1,6)	1:3:A:MET:HA	1:5:A:PHE:HD1	2	3.27
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	8	3.25
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	8	3.25
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	6	3.22
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	6	3.22
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	9	3.21
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	9	3.21
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	9	3.15
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	2	3.13
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	3	3.13
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	1	3.1
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	4	3.08
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	1	3.07
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	10	3.07
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	7	3.03
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	1	2.99
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	10	2.98
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	10	2.98
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	10	2.98
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	1	2.98
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	1	2.98
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	4	2.96
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	10	2.95
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	5	2.95
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	6	2.95
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	7	2.92
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	7	2.91
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	10	2.87
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	5	2.84
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	5	2.84
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	1	2.82
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	2	2.82
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	10	2.82
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	4	2.81
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	10	2.79
(1,607)	1:46:A:TYR:HD2	1:64:A:ARG:HA	10	2.79
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	10	2.78
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	10	2.78
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	4	2.77
(1,610)	1:46:A:TYR:HE2	1:64:A:ARG:HA	4	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	9	2.76
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	9	2.76
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	2	2.75
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	2	2.71
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	2	2.71
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	4	2.71
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	4	2.7
(1,608)	1:46:A:TYR:HD2	1:66:A:PHE:H	5	2.68
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	1	2.67
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	1	2.67
(1,608)	1:46:A:TYR:HD2	1:66:A:PHE:H	4	2.66
(1,51)	1:5:A:PHE:HD2	1:46:A:TYR:HE1	5	2.66
(1,608)	1:46:A:TYR:HD2	1:66:A:PHE:H	10	2.65
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB2	8	2.65
(1,49)	1:5:A:PHE:HD2	1:15:A:ASP:HB3	8	2.65
(1,610)	1:46:A:TYR:HE2	1:64:A:ARG:HA	10	2.64
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	4	2.64
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	4	2.64
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	5	2.63
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	2	2.62
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	5	2.61
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	7	2.61
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	7	2.61
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	7	2.61
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	8	2.61
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	8	2.61
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	7	2.61
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	7	2.61
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	5	2.6
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	5	2.6
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	5	2.6
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	5	2.58
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	10	2.55
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	10	2.53
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	1	2.52
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	8	2.5
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	8	2.5
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	8	2.5
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	2	2.47
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	10	2.47
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	7	2.47
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	10	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:37:A:THR:HA	1:46:A:TYR:HD1	5	2.46
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	1	2.43
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	2	2.42
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	10	2.41
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	8	2.4
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	8	2.4
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	8	2.4
(1,10)	1:3:A:MET:HG2	1:5:A:PHE:HE1	2	2.4
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	5	2.39
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	5	2.39
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	5	2.39
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	6	2.39
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	6	2.39
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	5	2.37
(1,607)	1:46:A:TYR:HD2	1:64:A:ARG:HA	4	2.37
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	1	2.37
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	1	2.37
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	3	2.37
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	3	2.37
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	5	2.35
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	2	2.34
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	2	2.34
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	2	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	1	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	1	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	1	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	4	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	4	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	4	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	7	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	7	2.34
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	7	2.34
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	10	2.34
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	5	2.33
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	4	2.33
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	4	2.32
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	4	2.31
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	6	2.31
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	6	2.31
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	6	2.31
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	5	2.31
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	5	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	5	2.31
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	10	2.3
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	10	2.3
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	10	2.3
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	5	2.29
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	4	2.29
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	4	2.29
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	2	2.29
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	2	2.29
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	2	2.29
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	7	2.29
(1,137)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	5	2.28
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	5	2.26
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	5	2.26
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	7	2.26
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	5	2.26
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	5	2.25
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	5	2.24
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	9	2.24
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	9	2.24
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	9	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	4	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	4	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	4	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	9	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	9	2.24
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	9	2.24
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	4	2.23
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	7	2.23
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	7	2.23
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	7	2.23
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	7	2.23
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	7	2.23
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	7	2.22
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	10	2.22
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	10	2.22
(1,482)	1:37:A:THR:HA	1:46:A:TYR:HD1	10	2.22
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	1	2.22
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	1	2.22
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	1	2.22
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	5	2.22
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	5	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	6	2.19
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	6	2.19
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	6	2.19
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	6	2.19
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	6	2.19
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	6	2.19
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	4	2.19
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	4	2.19
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	5	2.19
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	10	2.19
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	10	2.18
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	10	2.18
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	10	2.18
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	1	2.18
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	2	2.17
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	8	2.16
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	2	2.16
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	4	2.15
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	1	2.13
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	1	2.13
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	1	2.13
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	2	2.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	7	2.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	7	2.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	7	2.13
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	4	2.13
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	10	2.12
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	10	2.12
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	10	2.12
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	4	2.12
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	1	2.11
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	10	2.11
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	10	2.11
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	6	2.09
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	6	2.09
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	6	2.09
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	8	2.09
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	2	2.08
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	2	2.08
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	1	2.08
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	9	2.08
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	5	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	5	2.08
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	5	2.08
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	5	2.08
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	9	2.08
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	9	2.08
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	3	2.08
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	3	2.08
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	3	2.08
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	5	2.08
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	5	2.08
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	5	2.08
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	10	2.07
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	10	2.07
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	10	2.07
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	10	2.07
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	10	2.07
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	10	2.07
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	2	2.07
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	2	2.07
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	2	2.07
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	8	2.06
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	7	2.05
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	7	2.05
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	7	2.05
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	7	2.05
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	5	2.04
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	4	2.04
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	4	2.04
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	4	2.04
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	5	2.03
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	1	2.02
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	7	2.01
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	7	2.01
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	8	2.01
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	5	2.01
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	8	2.0
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	8	2.0
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	8	2.0
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	8	2.0
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	1	2.0
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	1	2.0
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	4	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	4	2.0
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	10	1.99
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	5	1.99
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	5	1.99
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	5	1.99
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	3	1.99
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	3	1.99
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	3	1.99
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	9	1.98
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	3	1.98
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	3	1.98
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	3	1.98
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	8	1.97
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	9	1.96
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	9	1.96
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	9	1.96
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	3	1.96
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	7	1.96
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	2	1.96
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	4	1.95
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	4	1.95
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	4	1.95
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	2	1.95
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	6	1.94
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	1	1.93
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	1	1.93
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	1	1.93
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	6	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	5	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	5	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	5	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	5	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	5	1.93
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	5	1.93
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	3	1.93
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	3	1.93
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	3	1.93
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	8	1.93
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	7	1.93
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	4	1.92
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	2	1.92
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	1	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	1	1.92
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	1	1.92
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	9	1.92
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	9	1.92
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	9	1.92
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	2	1.92
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	2	1.92
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	9	1.91
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	9	1.91
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	9	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	8	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	8	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	8	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	8	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	8	1.91
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	8	1.91
(1,140)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	10	1.91
(1,896)	1:62:A:LEU:HG	1:66:A:PHE:HE2	3	1.9
(1,149)	1:15:A:ASP:HB2	1:66:A:PHE:HZ	2	1.9
(1,149)	1:15:A:ASP:HB3	1:66:A:PHE:HZ	2	1.9
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	10	1.89
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	10	1.89
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	10	1.89
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	2	1.89
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	2	1.89
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	2	1.89
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	2	1.89
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	2	1.89
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	10	1.89
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	10	1.88
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	7	1.88
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	8	1.88
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	10	1.88
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	7	1.88
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	3	1.88
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	3	1.88
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	2	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	4	1.87
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	4	1.87
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	4	1.87
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	4	1.87
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	4	1.87
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	4	1.87
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	2	1.87
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	2	1.87
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	1	1.86
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	1	1.86
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	1	1.86
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	4	1.85
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	4	1.85
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	4	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	3	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	3	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	3	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	3	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	3	1.85
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	3	1.85
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	2	1.84
(1,202)	1:18:A:ARG:HB2	1:66:A:PHE:HE1	2	1.84
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	4	1.83
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	4	1.83
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	4	1.83
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	10	1.83
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	10	1.83
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	10	1.83
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	7	1.83
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	10	1.82
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	10	1.82
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	3	1.82
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	1	1.81
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	1	1.81
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	1	1.81
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	1	1.81
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	1	1.81
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	6	1.8
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	6	1.8
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	6	1.8
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	7	1.8
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	7	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	3	1.79
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	9	1.79
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	9	1.79
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	9	1.79
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	5	1.79
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	5	1.79
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	7	1.79
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	6	1.78
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	6	1.78
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	6	1.78
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	3	1.78
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	8	1.78
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	8	1.78
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	8	1.78
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	5	1.77
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	5	1.77
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	5	1.77
(1,117)	1:14:A:PRO:HG2	1:16:A:ALA:H	3	1.77
(1,37)	1:5:A:PHE:HA	1:66:A:PHE:HE1	4	1.77
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	1	1.77
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	4	1.76
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	4	1.76
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	4	1.76
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	1	1.76
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	1	1.76
(1,895)	1:62:A:LEU:HG	1:66:A:PHE:HD2	1	1.75
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	6	1.75
(1,142)	1:15:A:ASP:HB2	1:18:A:ARG:HB2	5	1.75
(1,142)	1:15:A:ASP:HB3	1:18:A:ARG:HB2	5	1.75
(1,140)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	4	1.75
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	10	1.75
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	7	1.74
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	7	1.74
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	7	1.74
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	5	1.74
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	5	1.74
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	5	1.74
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	1	1.74
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	1	1.74
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	1	1.74
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	1	1.74
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	1	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	1	1.74
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	5	1.73
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	7	1.73
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	7	1.73
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	7	1.73
(1,483)	1:37:A:THR:HA	1:46:A:TYR:HE1	5	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	6	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	6	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	6	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	6	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	6	1.73
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	6	1.73
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	6	1.73
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	8	1.72
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	7	1.72
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	10	1.71
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	10	1.71
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	10	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	8	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	8	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	8	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	8	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	8	1.71
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	8	1.71
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	8	1.71
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	8	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	6	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	6	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	6	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	6	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	6	1.71
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	6	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	3	1.71
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	3	1.71
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	3	1.71
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	3	1.71
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	8	1.71
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	8	1.71
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	9	1.71
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	9	1.71
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	3	1.7
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	10	1.69
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	9	1.69
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	4	1.69
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	2	1.69
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	8	1.69
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	7	1.68
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	8	1.68
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	8	1.68
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	8	1.68
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	5	1.68
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	5	1.68
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	5	1.68
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	6	1.68
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	8	1.68
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	9	1.68
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	10	1.68
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	9	1.67
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	9	1.67
(1,482)	1:37:A:THR:HA	1:46:A:TYR:HD1	4	1.67
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	5	1.67
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	5	1.67
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	5	1.67
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	5	1.67
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	5	1.67
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	5	1.67
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	4	1.67
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	1	1.67
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	3	1.67
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	7	1.67
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	7	1.67
(1,52)	1:5:A:PHE:HD2	1:66:A:PHE:HZ	3	1.67
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	10	1.66
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	10	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	10	1.66
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	10	1.66
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	10	1.66
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	10	1.66
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	1	1.66
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	5	1.66
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	5	1.66
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	6	1.65
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	6	1.65
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	6	1.65
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	6	1.65
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	6	1.65
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	6	1.65
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	6	1.65
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	2	1.65
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	10	1.65
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	2	1.64
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	5	1.64
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	5	1.64
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	5	1.64
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	6	1.63
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	2	1.63
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	3	1.63
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	3	1.63
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	8	1.63
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	9	1.63
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	8	1.62
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	8	1.62
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	8	1.62
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	7	1.62
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	7	1.62
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	1	1.61
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	1	1.61
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	1	1.61
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	1	1.61
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	1	1.61
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	1	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	1	1.61
(1,483)	1:37:A:THR:HA	1:46:A:TYR:HE1	10	1.6
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	10	1.59
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	10	1.59
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	10	1.59
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	8	1.59
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	8	1.59
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	8	1.59
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	5	1.59
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	5	1.59
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	2	1.58
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	2	1.57
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	5	1.57
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	6	1.56
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	1	1.56
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	1	1.56
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	1	1.56
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	1	1.56
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	1	1.56
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	1	1.56
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	1	1.56
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	7	1.56
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	7	1.56
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	7	1.56
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	7	1.56
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	7	1.56
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	7	1.56
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	10	1.56
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	5	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG21	3	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG22	3	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG23	3	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG21	4	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG22	4	1.56
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG23	4	1.56
(1,890)	1:62:A:LEU:HB3	1:66:A:PHE:HD2	9	1.55
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	6	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	6	1.55
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	6	1.55
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	5	1.55
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	5	1.55
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	5	1.55
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	2	1.55
(1,142)	1:15:A:ASP:HB2	1:18:A:ARG:HB2	10	1.55
(1,142)	1:15:A:ASP:HB3	1:18:A:ARG:HB2	10	1.55
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	10	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	10	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	10	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	10	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	10	1.54
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	10	1.54
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	10	1.54
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	2	1.53
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	2	1.53
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	2	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	1	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	1	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	1	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	1	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	1	1.53
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	1	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	3	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	3	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	3	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	3	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	3	1.53
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	3	1.53
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	9	1.53
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	7	1.52
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	1	1.52
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	1	1.52
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	2	1.51
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	10	1.51
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	10	1.51
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	10	1.51
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	10	1.51
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	10	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	10	1.51
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	10	1.51
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	10	1.51
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	10	1.51
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	10	1.51
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	9	1.51
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	9	1.51
(1,901)	1:62:A:LEU:HD11	1:66:A:PHE:HD2	1	1.5
(1,901)	1:62:A:LEU:HD12	1:66:A:PHE:HD2	1	1.5
(1,901)	1:62:A:LEU:HD13	1:66:A:PHE:HD2	1	1.5
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	7	1.5
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	7	1.5
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	7	1.5
(1,123)	1:15:A:ASP:H	1:18:A:ARG:HG2	7	1.5
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	2	1.49
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	1	1.49
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	1	1.49
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	1	1.49
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	1	1.49
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	9	1.49
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	6	1.48
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	10	1.48
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	10	1.48
(1,147)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	10	1.48
(1,147)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	10	1.48
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	8	1.48
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	8	1.48
(1,559)	1:44:A:ALA:HB1	1:69:A:LEU:HG	4	1.47
(1,559)	1:44:A:ALA:HB2	1:69:A:LEU:HG	4	1.47
(1,559)	1:44:A:ALA:HB3	1:69:A:LEU:HG	4	1.47
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	8	1.47
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	8	1.47
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	8	1.47
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	4	1.47
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	8	1.46
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	5	1.46
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	5	1.46
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	5	1.46
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	9	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	9	1.46
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	9	1.46
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	4	1.46
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	4	1.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	4	1.44
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	4	1.44
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	4	1.44
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	4	1.44
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	4	1.44
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	4	1.44
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	6	1.44
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	10	1.44
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	3	1.43
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	3	1.43
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	10	1.42
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	6	1.42
(1,147)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	5	1.42
(1,147)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	5	1.42
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	10	1.42
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	3	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	9	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	9	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	9	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	9	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	9	1.41
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	9	1.41
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	4	1.41
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	8	1.41
(1,142)	1:15:A:ASP:HB2	1:18:A:ARG:HB2	4	1.41
(1,142)	1:15:A:ASP:HB3	1:18:A:ARG:HB2	4	1.41
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	6	1.41
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	6	1.41
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	8	1.41
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	3	1.41
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	4	1.4
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	10	1.4
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	10	1.4
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	1	1.4
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	7	1.4
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	7	1.4
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	7	1.4
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	7	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	1	1.39
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	1	1.39
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	1	1.39
(1,147)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	4	1.39
(1,147)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	4	1.39
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	8	1.38
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	6	1.38
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	7	1.38
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	8	1.38
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	3	1.38
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	3	1.38
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	3	1.38
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	6	1.38
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	6	1.38
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	6	1.38
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	4	1.37
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	10	1.37
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	3	1.37
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	3	1.37
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	9	1.37
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	9	1.37
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	9	1.37
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	9	1.37
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	9	1.37
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	9	1.37
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	9	1.37
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	6	1.37
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	1	1.37
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	1	1.37
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	4	1.37
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	4	1.37
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	9	1.37
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	9	1.37
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	1	1.36
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	3	1.36
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	9	1.36
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	9	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	9	1.36
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	9	1.36
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	9	1.36
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	9	1.36
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	1	1.36
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	8	1.35
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	2	1.35
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	2	1.35
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	2	1.35
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	2	1.35
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	2	1.35
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	2	1.35
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	8	1.35
(1,540)	1:44:A:ALA:H	1:69:A:LEU:HG	10	1.35
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	4	1.35
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB2	4	1.35
(1,54)	1:5:A:PHE:HE1	1:65:A:ASP:HB3	4	1.35
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	2	1.34
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	2	1.34
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	2	1.34
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	7	1.34
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	7	1.34
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	4	1.34
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	10	1.34
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	10	1.34
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	10	1.34
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	10	1.34
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	1	1.34
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	1	1.34
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	1	1.34
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	1	1.34
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	1	1.34
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	1	1.34
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	5	1.34
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	6	1.34
(1,556)	1:44:A:ALA:HB1	1:61:A:HIS:HD2	7	1.33
(1,556)	1:44:A:ALA:HB2	1:61:A:HIS:HD2	7	1.33
(1,556)	1:44:A:ALA:HB3	1:61:A:HIS:HD2	7	1.33
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	3	1.33
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	9	1.33
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	9	1.32
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	8	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	2	1.31
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	2	1.31
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	2	1.31
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	4	1.31
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	4	1.31
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	4	1.31
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	8	1.31
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	1	1.3
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	3	1.3
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	6	1.3
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	9	1.3
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	9	1.3
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	9	1.3
(1,250)	1:20:A:ARG:HB2	1:49:A:LEU:H	7	1.3
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	1	1.3
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	3	1.3
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	8	1.3
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	4	1.29
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	4	1.29
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	1	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	7	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	7	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	7	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	7	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	7	1.29
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	7	1.29
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	6	1.29
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	6	1.29
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	6	1.29
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	6	1.29
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	6	1.29
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	6	1.29
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	4	1.28
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	7	1.28
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	7	1.28
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	7	1.28
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	7	1.28
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	7	1.28
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	7	1.28
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	5	1.28
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	2	1.28
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	2	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	2	1.28
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	6	1.28
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	6	1.28
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	6	1.28
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	2	1.28
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	3	1.28
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	1	1.28
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	8	1.27
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	8	1.27
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	8	1.27
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	7	1.27
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	7	1.27
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	1	1.27
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	2	1.27
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	2	1.27
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	2	1.27
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	6	1.27
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	6	1.27
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	6	1.27
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	4	1.26
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	4	1.26
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	4	1.26
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	4	1.26
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	4	1.26
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	4	1.26
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	4	1.26
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	7	1.26
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	7	1.26
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	8	1.26
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	6	1.26
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD2	7	1.26
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD3	7	1.26
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	10	1.25
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	5	1.25
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	5	1.25
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	5	1.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	5	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	5	1.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	5	1.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	5	1.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	5	1.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	5	1.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	5	1.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	5	1.25
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD3	9	1.25
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD3	9	1.25
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD3	9	1.25
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD3	9	1.25
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD3	9	1.25
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD2	9	1.25
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD3	9	1.25
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	2	1.25
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	2	1.25
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	2	1.25
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	5	1.25
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	2	1.24
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	2	1.24
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	2	1.24
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	2	1.24
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	7	1.24
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	9	1.24
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	9	1.23
(1,581)	1:46:A:TYR:HA	1:46:A:TYR:HD1	10	1.23
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	5	1.23
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	5	1.23
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	2	1.23
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	2	1.23
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	2	1.23
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	6	1.23
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	4	1.22
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	4	1.22
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	9	1.22
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	9	1.22
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	5	1.22
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	6	1.22
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	6	1.22
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	6	1.22
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	3	1.21
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	3	1.21
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	10	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	3	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	3	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	3	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	3	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	3	1.21
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	3	1.21
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	3	1.21
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	1	1.21
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	1	1.21
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	1	1.21
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	1	1.21
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	1	1.21
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	1	1.21
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	1	1.21
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	8	1.21
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	1	1.21
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	1	1.21
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	1	1.21
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	10	1.21
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	10	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	10	1.21
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	4	1.21
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	5	1.2
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	5	1.2
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	6	1.2
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	6	1.2
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	6	1.2
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	8	1.2
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	8	1.2
(1,208)	1:18:A:ARG:HG2	1:19:A:ALA:HA	3	1.2
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	9	1.2
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	5	1.19
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	7	1.19
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	7	1.19
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	7	1.19
(1,123)	1:15:A:ASP:H	1:18:A:ARG:HG2	5	1.19
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	6	1.18
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	2	1.18
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	2	1.18
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	3	1.18
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	3	1.18
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	2	1.18
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	10	1.17
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	10	1.17
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	2	1.17
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	2	1.17
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	2	1.17
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	2	1.17
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	6	1.17
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	6	1.17
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	6	1.17
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	6	1.17
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	6	1.17
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	6	1.17
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	10	1.17
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	10	1.17
(1,137)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	10	1.17
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	7	1.17
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	7	1.16
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	8	1.16
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	8	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	8	1.16
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	8	1.16
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	8	1.16
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	8	1.16
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	8	1.16
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	8	1.16
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	8	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	6	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	6	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	6	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	6	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	6	1.16
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	6	1.16
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	6	1.16
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	7	1.16
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	9	1.16
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	3	1.15
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	10	1.15
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	3	1.15
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	4	1.15
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	4	1.15
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	4	1.15
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	9	1.15
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	9	1.15
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	5	1.15
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	5	1.15
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	9	1.15
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	5	1.15
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	3	1.15
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	3	1.15
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	3	1.15
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	5	1.14
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	5	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	5	1.14
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	1	1.14
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	1	1.14
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	8	1.14
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	8	1.14
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	8	1.14
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	8	1.14
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	8	1.14
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	8	1.14
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	8	1.14
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	8	1.14
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	8	1.14
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	8	1.14
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	8	1.14
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	8	1.14
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	2	1.14
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	1	1.13
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	3	1.13
(1,556)	1:44:A:ALA:HB1	1:61:A:HIS:HD2	6	1.13
(1,556)	1:44:A:ALA:HB2	1:61:A:HIS:HD2	6	1.13
(1,556)	1:44:A:ALA:HB3	1:61:A:HIS:HD2	6	1.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD21	10	1.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD22	10	1.13
(1,252)	1:20:A:ARG:HB2	1:49:A:LEU:HD23	10	1.13
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	3	1.13
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	3	1.13
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	3	1.13
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	4	1.13
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	4	1.13
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	9	1.12
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	9	1.12
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	9	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	9	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	9	1.12
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	9	1.12
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	5	1.12
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	5	1.12
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	5	1.12
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	7	1.12
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	3	1.12
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	3	1.12
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	2	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	3	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	3	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	3	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	3	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	3	1.12
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	3	1.12
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	3	1.12
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	3	1.12
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	8	1.12
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	1	1.11
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	1	1.11
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	1	1.11
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	8	1.11
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	8	1.11
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	8	1.11
(1,604)	1:46:A:TYR:HD1	1:47:A:GLY:H	10	1.11
(1,585)	1:46:A:TYR:HB2	1:46:A:TYR:HD2	10	1.11
(1,513)	1:38:A:GLU:HG2	1:46:A:TYR:HA	9	1.11
(1,513)	1:38:A:GLU:HG3	1:46:A:TYR:HA	9	1.11
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	3	1.11
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	3	1.11
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	3	1.11
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	3	1.11
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	3	1.11
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	3	1.11
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	8	1.11
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	8	1.11
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	1	1.11
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	1	1.11
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	1	1.11
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	9	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	9	1.11
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	6	1.11
(1,974)	1:67:A:ARG:HG2	1:68:A:VAL:HB	4	1.1
(1,974)	1:67:A:ARG:HG3	1:68:A:VAL:HB	4	1.1
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	2	1.1
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	2	1.1
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	2	1.1
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	5	1.1
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	5	1.1
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	5	1.1
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	5	1.1
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	5	1.1
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	5	1.1
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	3	1.1
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	3	1.1
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	3	1.1
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	4	1.1
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	4	1.09
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	7	1.09
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	9	1.09
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	9	1.09
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	9	1.09
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	9	1.09
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	8	1.09
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	8	1.09
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	8	1.09
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	8	1.09
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	8	1.09
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	8	1.09
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	5	1.09
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	3	1.09
(1,217)	1:19:A:ALA:H	1:66:A:PHE:HE1	2	1.09
(1,137)	1:15:A:ASP:HB2	1:46:A:TYR:HE1	4	1.09
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	4	1.09
(1,919)	1:63:A:ASP:HB2	1:64:A:ARG:HG3	4	1.08
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	9	1.08
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	10	1.08
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	6	1.08
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	6	1.08
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	3	1.08
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	8	1.08
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	9	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	9	1.08
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	9	1.08
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	9	1.08
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	9	1.08
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	9	1.08
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	2	1.08
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	2	1.08
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	6	1.08
(1,585)	1:46:A:TYR:HB2	1:46:A:TYR:HD2	5	1.08
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	3	1.08
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	3	1.08
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	3	1.08
(1,143)	1:15:A:ASP:HB2	1:18:A:ARG:HG2	7	1.08
(1,143)	1:15:A:ASP:HB3	1:18:A:ARG:HG2	7	1.08
(1,143)	1:15:A:ASP:HB2	1:18:A:ARG:HG3	7	1.08
(1,143)	1:15:A:ASP:HB3	1:18:A:ARG:HG3	7	1.08
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	10	1.08
(1,123)	1:15:A:ASP:H	1:18:A:ARG:HG2	10	1.08
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	8	1.08
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	10	1.08
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	2	1.07
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	2	1.07
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	2	1.07
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	2	1.07
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	2	1.07
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	2	1.07
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	10	1.07
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	3	1.07
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	3	1.07
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	3	1.07
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	3	1.07
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	3	1.07
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	3	1.07
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	3	1.07
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	6	1.07
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	6	1.07
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	6	1.07
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	10	1.07
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	7	1.07
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	9	1.07
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	9	1.07
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	10	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	10	1.06
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	10	1.06
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	10	1.06
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	10	1.06
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	10	1.06
(1,779)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	6	1.06
(1,779)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	6	1.06
(1,779)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	6	1.06
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	4	1.06
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	4	1.06
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	4	1.06
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	4	1.06
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	1	1.06
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	1	1.06
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	1	1.06
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	2	1.06
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	6	1.06
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	6	1.06
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	6	1.06
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	4	1.06
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG11	4	1.05
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG12	4	1.05
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG13	4	1.05
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG21	4	1.05
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG22	4	1.05
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG23	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG11	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG12	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG13	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG21	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG22	4	1.05
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG23	4	1.05
(1,954)	1:65:A:ASP:HB2	1:67:A:ARG:HA	8	1.05
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	4	1.05
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	4	1.05
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	4	1.05
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	6	1.05
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	6	1.05
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	6	1.05
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	7	1.05
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	7	1.05
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	7	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	1	1.05
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	6	1.05
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	7	1.05
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	2	1.05
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	2	1.05
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	2	1.05
(1,585)	1:46:A:TYR:HB2	1:46:A:TYR:HD2	4	1.05
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	10	1.05
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	10	1.05
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	10	1.05
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	8	1.05
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	8	1.05
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	3	1.05
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	5	1.05
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	5	1.05
(1,46)	1:5:A:PHE:HB3	1:66:A:PHE:HE1	6	1.05
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	5	1.04
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	5	1.04
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	5	1.04
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	5	1.04
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	8	1.04
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	8	1.04
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	8	1.04
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	5	1.04
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	3	1.04
(1,811)	1:59:A:GLU:HG3	1:74:A:ALA:HA	2	1.04
(1,604)	1:46:A:TYR:HD1	1:47:A:GLY:H	5	1.04
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	5	1.04
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	7	1.04
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	2	1.04
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	5	1.04
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	5	1.04
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	5	1.04
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	5	1.04
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	5	1.04
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	5	1.04
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	2	1.04
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	2	1.04
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	2	1.04
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	2	1.04
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	2	1.04
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	2	1.04
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	2	1.04
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	2	1.04
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	2	1.04
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	2	1.04
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	2	1.04
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	7	1.04
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	7	1.04
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	8	1.04
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	10	1.04
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	10	1.04
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	3	1.04
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	3	1.04
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	3	1.04
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	7	1.04
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	2	1.04
(1,954)	1:65:A:ASP:HB2	1:67:A:ARG:HA	3	1.03
(1,951)	1:65:A:ASP:HA	1:66:A:PHE:HD1	4	1.03
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	7	1.03
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	3	1.03
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	3	1.03
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	3	1.03
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	2	1.03
(1,891)	1:62:A:LEU:HB3	1:66:A:PHE:HE2	9	1.03
(1,808)	1:59:A:GLU:HG2	1:74:A:ALA:HA	6	1.03
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	5	1.03
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	5	1.03
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	10	1.03
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	5	1.03
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	2	1.03
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	5	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	1	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	1	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	1	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	10	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	10	1.03
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	10	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	4	1.03
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	4	1.03
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	4	1.03
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	7	1.03
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	10	1.03
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	1	1.02
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	4	1.02
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	9	1.02
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	10	1.02
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	9	1.02
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	9	1.02
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	9	1.02
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	7	1.02
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	7	1.02
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	3	1.02
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	3	1.02
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	3	1.02
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	3	1.02
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	3	1.02
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	3	1.02
(1,604)	1:46:A:TYR:HD1	1:47:A:GLY:H	4	1.02
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	8	1.02
(1,600)	1:46:A:TYR:HB3	1:62:A:LEU:HG	5	1.02
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	2	1.02
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	8	1.02
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	3	1.02
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	3	1.02
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	3	1.02
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	3	1.02
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	3	1.02
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	3	1.02
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	4	1.02
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	4	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	4	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	4	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	4	1.02
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	4	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	4	1.02
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	8	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	8	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	8	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	8	1.02
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	8	1.02
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	8	1.02
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	8	1.02
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	1	1.02
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	10	1.02
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB1	3	1.02
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB2	3	1.02
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB3	3	1.02
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	8	1.02
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	6	1.02
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	6	1.02
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	10	1.02
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	10	1.02
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	8	1.02
(1,919)	1:63:A:ASP:HB2	1:64:A:ARG:HG3	3	1.01
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	3	1.01
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	8	1.01
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	8	1.01
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD21	2	1.01
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD22	2	1.01
(1,626)	1:47:A:GLY:HA3	1:62:A:LEU:HD23	2	1.01
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	9	1.01
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	9	1.01
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	9	1.01
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	9	1.01
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	9	1.01
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	9	1.01
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	3	1.01
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	3	1.01
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	3	1.01
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	3	1.01
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	3	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	3	1.01
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	3	1.01
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	3	1.01
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	3	1.01
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	3	1.01
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	3	1.01
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	3	1.01
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	10	1.01
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	8	1.01
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	8	1.01
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	8	1.01
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	6	1.01
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	6	1.01
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	10	1.01
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	8	1.01
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	5	1.01
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	8	1.0
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	4	1.0
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	4	1.0
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	4	1.0
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	3	1.0
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	10	1.0
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	5	1.0
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	5	1.0
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	5	1.0
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	5	1.0
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	5	1.0
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	5	1.0
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	7	1.0
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	7	1.0
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	7	1.0
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	5	1.0
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	5	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	4	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	4	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	4	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	4	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	4	1.0
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	4	1.0
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	4	1.0
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	4	1.0
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	4	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	4	1.0
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	4	1.0
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	4	1.0
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	4	1.0
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	1	1.0
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	1	1.0
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	1	1.0
(1,897)	1:62:A:LEU:HG	1:66:A:PHE:HZ	6	0.99
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	5	0.99
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	3	0.99
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	3	0.99
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	3	0.99
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	3	0.99
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	3	0.99
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	3	0.99
(1,811)	1:59:A:GLU:HG3	1:74:A:ALA:HA	8	0.99
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	2	0.99
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	2	0.99
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	3	0.98
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	1	0.98
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	1	0.98
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	3	0.98
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	9	0.98
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	9	0.98
(1,483)	1:37:A:THR:HA	1:46:A:TYR:HE1	4	0.98
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	4	0.98
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	4	0.98
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	4	0.98
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD2	9	0.98
(1,399)	1:28:A:PRO:HG2	1:53:A:PRO:HD3	9	0.98
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD2	9	0.98
(1,399)	1:28:A:PRO:HG3	1:53:A:PRO:HD3	9	0.98
(1,907)	1:62:A:LEU:HD21	1:70:A:ASP:H	9	0.97
(1,907)	1:62:A:LEU:HD22	1:70:A:ASP:H	9	0.97
(1,907)	1:62:A:LEU:HD23	1:70:A:ASP:H	9	0.97
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	4	0.97
(1,811)	1:59:A:GLU:HG3	1:74:A:ALA:HA	10	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	4	0.97
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	4	0.97
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	10	0.97
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	2	0.97
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	4	0.97
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	5	0.97
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	5	0.97
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	1	0.97
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	1	0.97
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	1	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	1	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	2	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	2	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	2	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	2	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	2	0.97
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	2	0.97
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	2	0.97
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	4	0.97
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	4	0.97
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD21	8	0.97
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD22	8	0.97
(1,267)	1:20:A:ARG:HG3	1:49:A:LEU:HD23	8	0.97
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	6	0.97
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	8	0.97
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	3	0.97
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	8	0.96
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	2	0.96
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	8	0.96
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	8	0.96
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	8	0.96
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	6	0.96
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	6	0.96
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	6	0.96
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	6	0.96
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	6	0.96
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	6	0.96
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	9	0.96
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	10	0.96
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	10	0.96
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	10	0.96
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	10	0.96
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	10	0.96
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	10	0.96
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	4	0.96
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	4	0.96
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	4	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG11	1	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG12	1	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG13	1	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG21	1	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG22	1	0.96
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG23	1	0.96
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	10	0.96
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	10	0.96
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	10	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	2	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	4	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	4	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	4	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	4	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	4	0.96
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	4	0.96
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	7	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:15:A:ASP:HB3	1:46:A:TYR:HE1	5	0.96
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	10	0.96
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	2	0.96
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	3	0.96
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	4	0.96
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	4	0.96
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	5	0.96
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	1	0.95
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	5	0.95
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	7	0.95
(1,22)	1:4:A:ALA:H	1:5:A:PHE:HE1	5	0.95
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	5	0.94
(1,883)	1:62:A:LEU:HB2	1:66:A:PHE:HE2	9	0.94
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	7	0.94
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	9	0.94
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	9	0.94
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	9	0.94
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	2	0.94
(1,742)	1:54:A:ASP:H	1:56:A:THR:HG21	4	0.94
(1,742)	1:54:A:ASP:H	1:56:A:THR:HG22	4	0.94
(1,742)	1:54:A:ASP:H	1:56:A:THR:HG23	4	0.94
(1,605)	1:46:A:TYR:HD1	1:66:A:PHE:HZ	8	0.94
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	2	0.94
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	8	0.94
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	4	0.94
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	4	0.94
(1,149)	1:15:A:ASP:HB2	1:66:A:PHE:HZ	6	0.94
(1,149)	1:15:A:ASP:HB3	1:66:A:PHE:HZ	6	0.94
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	6	0.94
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	7	0.93
(1,581)	1:46:A:TYR:HA	1:46:A:TYR:HD1	5	0.93
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	2	0.93
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	4	0.93
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	4	0.93
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	4	0.93
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	4	0.93
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	4	0.93
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	4	0.93
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	9	0.93
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	10	0.93
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	8	0.93
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	8	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	7	0.92
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	5	0.92
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	8	0.92
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	5	0.92
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	1	0.92
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	1	0.92
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	1	0.92
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	5	0.92
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	5	0.92
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	5	0.92
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	5	0.92
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	5	0.92
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	5	0.92
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	3	0.92
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	6	0.92
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	6	0.92
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	6	0.92
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	6	0.92
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	10	0.92
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	10	0.92
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	1	0.92
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	4	0.92
(1,202)	1:18:A:ARG:HB2	1:66:A:PHE:HE1	4	0.92
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	6	0.92
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	10	0.92
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	1	0.91
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	9	0.91
(1,807)	1:59:A:GLU:HG2	1:73:A:PRO:HA	6	0.91
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	7	0.91
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	7	0.91
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	7	0.91
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	7	0.91
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	7	0.91
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	7	0.91
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	7	0.91
(1,556)	1:44:A:ALA:HB1	1:61:A:HIS:HD2	8	0.91
(1,556)	1:44:A:ALA:HB2	1:61:A:HIS:HD2	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:44:A:ALA:HB3	1:61:A:HIS:HD2	8	0.91
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	1	0.91
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	1	0.91
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	1	0.91
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	10	0.91
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	2	0.91
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	1	0.91
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	1	0.91
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	7	0.91
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	6	0.9
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	6	0.9
(1,826)	1:60:A:VAL:HB	1:70:A:ASP:H	2	0.9
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	8	0.9
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	8	0.9
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	8	0.9
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	8	0.9
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	8	0.9
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	8	0.9
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	3	0.9
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	3	0.9
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	3	0.9
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	9	0.9
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	9	0.9
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	9	0.9
(1,473)	1:36:A:GLU:HG3	1:47:A:GLY:H	2	0.9
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	5	0.9
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	8	0.9
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	8	0.9
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	8	0.9
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	9	0.9
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	10	0.89
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	10	0.89
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	10	0.89
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	2	0.89
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	2	0.89
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	2	0.89
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	2	0.89
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	2	0.89
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	2	0.89
(1,581)	1:46:A:TYR:HA	1:46:A:TYR:HD1	4	0.89
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	2	0.89
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	7	0.89
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	10	0.89
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	8	0.89
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	8	0.89
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	8	0.89
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	5	0.89
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	5	0.89
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	5	0.89
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	7	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	3	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	3	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	3	0.88
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB1	6	0.88
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB2	6	0.88
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB3	6	0.88
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	6	0.88
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	6	0.88
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	6	0.88
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	6	0.88
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	6	0.88
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	6	0.88
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	1	0.88
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	6	0.88
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	10	0.88
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	1	0.88
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	2	0.88
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	2	0.88
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	2	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	2	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	2	0.88
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	2	0.88
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	7	0.88
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	7	0.88
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	7	0.88
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	7	0.88
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	7	0.88
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	7	0.88
(1,146)	1:15:A:ASP:HB2	1:37:A:THR:H	8	0.88
(1,146)	1:15:A:ASP:HB3	1:37:A:THR:H	8	0.88
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	9	0.88
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	4	0.88
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	7	0.87
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	7	0.87
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	9	0.87
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	6	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	1	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	1	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	1	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	1	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	1	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	1	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	6	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	6	0.87
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	6	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	6	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	6	0.87
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	6	0.87
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	1	0.87
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	1	0.87
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	10	0.87
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	10	0.87
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	2	0.87
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	2	0.87
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	2	0.87
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	2	0.87
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	2	0.87
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	2	0.87
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	7	0.87
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	7	0.87
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	2	0.86
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	2	0.86
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	2	0.86
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	10	0.86
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	10	0.86
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	10	0.86
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	4	0.86
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	4	0.86
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	4	0.86
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	4	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	4	0.86
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	4	0.86
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	4	0.86
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	3	0.86
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	3	0.86
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	3	0.86
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	3	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG11	1	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG12	1	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG13	1	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG21	1	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG22	1	0.86
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG23	1	0.86
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	5	0.86
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	5	0.86
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	5	0.86
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	4	0.86
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	7	0.86
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	4	0.86
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	5	0.86
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	5	0.86
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	8	0.86
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	4	0.85
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	4	0.85
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	4	0.85
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	6	0.85
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	10	0.85
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	10	0.85
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	10	0.85
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	10	0.85
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	10	0.85
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	10	0.85
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	7	0.85
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	7	0.85
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	7	0.85
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	7	0.85
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	7	0.85
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	7	0.85
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	9	0.85
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	9	0.85
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	9	0.85
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	9	0.85
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	9	0.85
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	1	0.85
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	5	0.85
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	3	0.85
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	3	0.85
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	3	0.85
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	2	0.85
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	2	0.85
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	6	0.85
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	6	0.85
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	6	0.85
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	6	0.85
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	6	0.85
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	6	0.85
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	9	0.85
(1,55)	1:5:A:PHE:HE1	1:66:A:PHE:H	4	0.85
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	7	0.85
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	3	0.84
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	3	0.84
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	3	0.84
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	7	0.84
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	10	0.84
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	9	0.84
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	1	0.84
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	1	0.84
(1,123)	1:15:A:ASP:H	1:18:A:ARG:HG2	4	0.84
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	3	0.84
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	10	0.84
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	6	0.83
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	7	0.83
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	3	0.83
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	8	0.83
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	10	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	7	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	7	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	7	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	7	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	7	0.83
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	7	0.83
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	7	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	7	0.83
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	1	0.83
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	1	0.83
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	1	0.83
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	9	0.83
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	3	0.83
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	3	0.83
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	3	0.83
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	6	0.83
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	1	0.83
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	6	0.82
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	6	0.82
(1,921)	1:63:A:ASP:HB2	1:69:A:LEU:HB2	2	0.82
(1,919)	1:63:A:ASP:HB2	1:64:A:ARG:HG3	9	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	5	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	5	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	5	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD21	6	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD22	6	0.82
(1,854)	1:61:A:HIS:HB3	1:62:A:LEU:HD23	6	0.82
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB1	10	0.82
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB2	10	0.82
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB3	10	0.82
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	2	0.82
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	2	0.82
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	10	0.82
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	10	0.82
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	10	0.82
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	10	0.82
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	10	0.82
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	10	0.82
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	7	0.82
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	10	0.82
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	10	0.82
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	10	0.82
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	10	0.82
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	10	0.82
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	10	0.82
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	7	0.82
(1,133)	1:15:A:ASP:HA	1:19:A:ALA:H	8	0.82
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	9	0.81
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	9	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	4	0.81
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	8	0.81
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	8	0.81
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	8	0.81
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	7	0.81
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	8	0.81
(1,535)	1:43:A:ALA:HB1	1:63:A:ASP:HB2	9	0.81
(1,535)	1:43:A:ALA:HB2	1:63:A:ASP:HB2	9	0.81
(1,535)	1:43:A:ALA:HB3	1:63:A:ASP:HB2	9	0.81
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	1	0.81
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	1	0.81
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	6	0.81
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	6	0.81
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	10	0.81
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	10	0.81
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	10	0.81
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	10	0.81
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	10	0.81
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	10	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	2	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	2	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	2	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	2	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	2	0.81
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	2	0.81
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	9	0.81
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	7	0.81
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	8	0.8
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	8	0.8
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	8	0.8
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	8	0.8
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	9	0.8
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	3	0.8
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD2	8	0.8
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD3	8	0.8
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD2	8	0.8
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD3	8	0.8
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD2	8	0.8
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD3	8	0.8
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD2	8	0.8
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD3	8	0.8
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD2	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD3	8	0.8
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD2	8	0.8
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD3	8	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	10	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	10	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	10	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	10	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	10	0.8
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	10	0.8
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	6	0.8
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	4	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	2	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	2	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	2	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	2	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	2	0.8
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	2	0.8
(1,149)	1:15:A:ASP:HB2	1:66:A:PHE:HZ	3	0.8
(1,149)	1:15:A:ASP:HB3	1:66:A:PHE:HZ	3	0.8
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	2	0.8
(1,21)	1:4:A:ALA:H	1:5:A:PHE:HD1	2	0.8
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	2	0.8
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	3	0.79
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	9	0.79
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	9	0.79
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	9	0.79
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	9	0.79
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	2	0.79
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	2	0.79
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	6	0.79
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	10	0.79
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	10	0.79
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD21	10	0.79
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD23	10	0.79
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD21	10	0.79
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD23	10	0.79
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD21	10	0.79
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD23	10	0.79
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD21	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD23	10	0.79
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD21	10	0.79
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD23	10	0.79
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD21	10	0.79
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD22	10	0.79
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD23	10	0.79
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	6	0.79
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	6	0.79
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	6	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	7	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	7	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	7	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	7	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	7	0.79
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	7	0.79
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	7	0.79
(1,379)	1:27:A:VAL:HB	1:51:A:THR:H	10	0.79
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	5	0.79
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	5	0.79
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	4	0.79
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	4	0.79
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	4	0.79
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	6	0.79
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	5	0.78
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	5	0.78
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	5	0.78
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	8	0.78
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	8	0.78
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	8	0.78
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	8	0.78
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	8	0.78
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	8	0.78
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	6	0.78
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	9	0.78
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	7	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	2	0.78
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	2	0.78
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	2	0.78
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	2	0.78
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	2	0.78
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	2	0.78
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	9	0.78
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	9	0.78
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	9	0.78
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	9	0.78
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	9	0.78
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	9	0.78
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	7	0.78
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	2	0.78
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	2	0.78
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	2	0.78
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	2	0.78
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	2	0.78
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	6	0.78
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	8	0.78
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	2	0.77
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	1	0.77
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB2	5	0.77
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB2	5	0.77
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB2	5	0.77
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB3	5	0.77
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB3	5	0.77
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB3	5	0.77
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB2	5	0.77
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB2	5	0.77
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB2	5	0.77
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB3	5	0.77
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB3	5	0.77
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB3	5	0.77
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	4	0.77
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	4	0.77
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD3	10	0.77
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD3	10	0.77
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD3	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD3	10	0.77
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD3	10	0.77
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD2	10	0.77
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD3	10	0.77
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	1	0.77
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	1	0.77
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	1	0.77
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	1	0.77
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	1	0.77
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	1	0.77
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	4	0.77
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	7	0.77
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	1	0.76
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	1	0.76
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	1	0.76
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	6	0.76
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	8	0.76
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	4	0.76
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	7	0.76
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	6	0.76
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	6	0.76
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	6	0.76
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	6	0.76
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	6	0.76
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:19:A:ALA:HA	1:66:A:PHE:HE2	2	0.76
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG11	6	0.75
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG12	6	0.75
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG13	6	0.75
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG21	6	0.75
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG22	6	0.75
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG23	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG11	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG12	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG13	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG21	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG22	6	0.75
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG23	6	0.75
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	7	0.75
(1,694)	1:51:A:THR:HG21	1:55:A:GLY:H	8	0.75
(1,694)	1:51:A:THR:HG22	1:55:A:GLY:H	8	0.75
(1,694)	1:51:A:THR:HG23	1:55:A:GLY:H	8	0.75
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	4	0.75
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	9	0.75
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	8	0.75
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	8	0.75
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	8	0.75
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	8	0.75
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB1	1	0.75
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB2	1	0.75
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB3	1	0.75
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	4	0.75
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB2	2	0.75
(1,57)	1:5:A:PHE:HE1	1:66:A:PHE:HB3	2	0.75
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	3	0.75
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	8	0.75
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	5	0.75
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	5	0.75
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	3	0.74
(1,919)	1:63:A:ASP:HB2	1:64:A:ARG:HG3	6	0.74
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	5	0.74
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	5	0.74
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	5	0.74
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	5	0.74
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	5	0.74
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	5	0.74
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	5	0.74
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	5	0.74
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	5	0.74
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	5	0.74
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	5	0.74
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	8	0.74
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	8	0.74
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	8	0.74
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	4	0.74
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	6	0.74
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	8	0.73
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	8	0.73
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	6	0.73
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	1	0.73
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	3	0.73
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	5	0.73
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	3	0.73
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	9	0.72
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	9	0.72
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	9	0.72
(1,906)	1:62:A:LEU:HD21	1:66:A:PHE:HE2	2	0.72
(1,906)	1:62:A:LEU:HD22	1:66:A:PHE:HE2	2	0.72
(1,906)	1:62:A:LEU:HD23	1:66:A:PHE:HE2	2	0.72
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB1	10	0.72
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB2	10	0.72
(1,813)	1:59:A:GLU:HB2	1:74:A:ALA:HB3	10	0.72
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB1	10	0.72
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB2	10	0.72
(1,813)	1:59:A:GLU:HB3	1:74:A:ALA:HB3	10	0.72
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	4	0.72
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	1	0.72
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	1	0.72
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	1	0.72
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	1	0.72
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	1	0.72
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	1	0.72
(1,573)	1:46:A:TYR:H	1:46:A:TYR:HD2	4	0.72
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	5	0.72
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	5	0.72
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD2	10	0.72
(1,396)	1:28:A:PRO:HB2	1:53:A:PRO:HD3	10	0.72
(1,135)	1:15:A:ASP:HB2	1:18:A:ARG:H	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB2	10	0.72
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB3	10	0.72
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	4	0.72
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	10	0.72
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	10	0.72
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	2	0.71
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	2	0.71
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	2	0.71
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	2	0.71
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	2	0.71
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	2	0.71
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	1	0.71
(1,802)	1:59:A:GLU:H	1:74:A:ALA:HA	2	0.71
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	1	0.71
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	1	0.71
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	5	0.71
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	5	0.71
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	5	0.71
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	5	0.71
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	5	0.71
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	5	0.71
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	8	0.71
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	5	0.71
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	10	0.71
(1,557)	1:44:A:ALA:HB1	1:62:A:LEU:H	8	0.71
(1,557)	1:44:A:ALA:HB2	1:62:A:LEU:H	8	0.71
(1,557)	1:44:A:ALA:HB3	1:62:A:LEU:H	8	0.71
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	9	0.71
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	9	0.71
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	10	0.71
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	10	0.71
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	10	0.71
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	8	0.71
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	8	0.71
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	8	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG11	10	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG12	10	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG13	10	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG21	10	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG22	10	0.71
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG23	10	0.71
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG11	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG12	7	0.71
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG13	7	0.71
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG21	7	0.71
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG22	7	0.71
(1,326)	1:24:A:VAL:HA	1:50:A:VAL:HG23	7	0.71
(1,311)	1:23:A:ALA:HB1	1:51:A:THR:H	4	0.71
(1,311)	1:23:A:ALA:HB2	1:51:A:THR:H	4	0.71
(1,311)	1:23:A:ALA:HB3	1:51:A:THR:H	4	0.71
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD2	9	0.71
(1,188)	1:18:A:ARG:H	1:18:A:ARG:HD3	9	0.71
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	7	0.71
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	4	0.7
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	9	0.7
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	4	0.7
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	7	0.7
(1,613)	1:46:A:TYR:HE2	1:66:A:PHE:H	2	0.7
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	6	0.7
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	7	0.7
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	2	0.7
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	2	0.7
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	2	0.7
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	5	0.7
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	5	0.7
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	5	0.7
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	8	0.7
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB1	3	0.7
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB2	3	0.7
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB3	3	0.7
(1,61)	1:6:A:ASP:H	1:7:A:GLY:H	4	0.7
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	7	0.7
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	1	0.7
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	6	0.7
(1,974)	1:67:A:ARG:HG2	1:68:A:VAL:HB	6	0.69
(1,974)	1:67:A:ARG:HG3	1:68:A:VAL:HB	6	0.69
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	6	0.69
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	6	0.69
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	6	0.69
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	5	0.69
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	1	0.69
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	10	0.69
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	3	0.69
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:46:A:TYR:HB2	1:62:A:LEU:HG	10	0.69
(1,573)	1:46:A:TYR:H	1:46:A:TYR:HD2	5	0.69
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	1	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	9	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	9	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	9	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	9	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	9	0.69
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	9	0.69
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	9	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	3	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	3	0.69
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	3	0.69
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	3	0.69
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	4	0.69
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	5	0.69
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	1	0.69
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	8	0.69
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	8	0.69
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	5	0.69
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	9	0.69
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	8	0.69
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	4	0.68
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	10	0.68
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	10	0.68
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	10	0.68
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	8	0.68
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	8	0.68
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	3	0.68
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	6	0.68
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	6	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	5	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	5	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	5	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	5	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	5	0.68
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	5	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	6	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	6	0.68
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	6	0.68
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	6	0.68
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	9	0.68
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	9	0.68
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	9	0.68
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	2	0.68
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	2	0.68
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	2	0.68
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB1	6	0.68
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB2	6	0.68
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB3	6	0.68
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	5	0.68
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	10	0.68
(1,41)	1:5:A:PHE:HB2	1:66:A:PHE:HE1	9	0.68
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	8	0.68
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	8	0.67
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	8	0.67
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	8	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	8	0.67
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	8	0.67
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	8	0.67
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	8	0.67
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	8	0.67
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	8	0.67
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	8	0.67
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	8	0.67
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	8	0.67
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	3	0.67
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	3	0.67
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	3	0.67
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	3	0.67
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	3	0.67
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	3	0.67
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	6	0.67
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	10	0.67
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	1	0.67
(1,56)	1:5:A:PHE:HE1	1:66:A:PHE:HA	3	0.67
(1,33)	1:5:A:PHE:H	1:66:A:PHE:HE1	9	0.67
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	9	0.67
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	5	0.66
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	10	0.66
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	10	0.66
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	1	0.66
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	7	0.66
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	7	0.66
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	7	0.66
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	7	0.66
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	7	0.66
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	7	0.66
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	7	0.66
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	6	0.66
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	6	0.66
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	6	0.66
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	9	0.66
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	9	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	7	0.66
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	6	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG11	5	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG12	5	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG13	5	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG21	5	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG22	5	0.65
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG23	5	0.65
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	9	0.65
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	9	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG11	2	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG12	2	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG13	2	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG21	2	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG22	2	0.65
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG23	2	0.65
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	1	0.65
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	1	0.65
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	1	0.65
(1,44)	1:5:A:PHE:HB3	1:5:A:PHE:HE2	2	0.65
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	3	0.65
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	9	0.64
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	1	0.64
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	8	0.64
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	9	0.64
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	4	0.64
(1,387)	1:27:A:VAL:HG11	1:50:A:VAL:HB	8	0.64
(1,387)	1:27:A:VAL:HG12	1:50:A:VAL:HB	8	0.64
(1,387)	1:27:A:VAL:HG13	1:50:A:VAL:HB	8	0.64
(1,387)	1:27:A:VAL:HG21	1:50:A:VAL:HB	8	0.64
(1,387)	1:27:A:VAL:HG22	1:50:A:VAL:HB	8	0.64
(1,387)	1:27:A:VAL:HG23	1:50:A:VAL:HB	8	0.64
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB1	2	0.64
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB2	2	0.64
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB3	2	0.64
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	7	0.64
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	4	0.64
(1,31)	1:5:A:PHE:H	1:5:A:PHE:HE1	2	0.64
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	4	0.63
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	4	0.63
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	4	0.63
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	4	0.63
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	4	0.63
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	9	0.63
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	7	0.63
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	5	0.63
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	5	0.63
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	5	0.63
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	5	0.63
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	5	0.63
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	5	0.63
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	7	0.63
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	3	0.63
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	4	0.63
(1,209)	1:18:A:ARG:HG2	1:20:A:ARG:H	7	0.63
(1,721)	1:52:A:ARG:HG2	1:56:A:THR:H	9	0.62
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	2	0.62
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	2	0.62
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	2	0.62
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	2	0.62
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	2	0.62
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	2	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	7	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	7	0.62
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	7	0.62
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	7	0.62
(1,639)	1:48:A:VAL:HG11	1:60:A:VAL:H	10	0.62
(1,639)	1:48:A:VAL:HG12	1:60:A:VAL:H	10	0.62
(1,639)	1:48:A:VAL:HG13	1:60:A:VAL:H	10	0.62
(1,639)	1:48:A:VAL:HG21	1:60:A:VAL:H	10	0.62
(1,639)	1:48:A:VAL:HG22	1:60:A:VAL:H	10	0.62
(1,639)	1:48:A:VAL:HG23	1:60:A:VAL:H	10	0.62
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	8	0.62
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	8	0.62
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	8	0.62
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	8	0.62
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	8	0.62
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	8	0.62
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	10	0.62
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	5	0.62
(1,506)	1:38:A:GLU:HB2	1:40:A:GLY:H	2	0.62
(1,506)	1:38:A:GLU:HB3	1:40:A:GLY:H	2	0.62
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	2	0.62
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	2	0.62
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	2	0.62
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	2	0.62
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	2	0.62
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	8	0.62
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	8	0.62
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	8	0.62
(1,125)	1:15:A:ASP:H	1:37:A:THR:H	2	0.62
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	9	0.62
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	4	0.62
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	6	0.61
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	5	0.61
(1,473)	1:36:A:GLU:HG3	1:47:A:GLY:H	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	10	0.61
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	10	0.61
(1,266)	1:20:A:ARG:HG3	1:49:A:LEU:H	8	0.61
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	5	0.61
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	5	0.61
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	5	0.61
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	2	0.61
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	2	0.61
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	2	0.61
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	10	0.61
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	8	0.61
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	3	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	3	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	3	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	4	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	4	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	4	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	6	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	6	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	6	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	9	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	9	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	9	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	10	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	10	0.6
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	10	0.6
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	7	0.6
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	7	0.6
(1,859)	1:61:A:HIS:HB3	1:69:A:LEU:HG	5	0.6
(1,857)	1:61:A:HIS:HB3	1:69:A:LEU:HA	9	0.6
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	4	0.6
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	3	0.6
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	4	0.6
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	6	0.6
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	4	0.6
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	4	0.6
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	4	0.6
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	4	0.6
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	4	0.6
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	4	0.6
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	7	0.6
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	10	0.6
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	1	0.6
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	4	0.6
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	4	0.6
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	4	0.6
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG11	1:30:A:GLY:HA3	10	0.6
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG12	1:30:A:GLY:HA3	10	0.6
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG13	1:30:A:GLY:HA3	10	0.6
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG21	1:30:A:GLY:HA3	10	0.6
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG22	1:30:A:GLY:HA3	10	0.6
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA2	10	0.6
(1,340)	1:24:A:VAL:HG23	1:30:A:GLY:HA3	10	0.6
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	4	0.6
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	4	0.6
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	3	0.6
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	10	0.6
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	8	0.6
(1,12)	1:3:A:MET:HG3	1:5:A:PHE:H	2	0.6
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	6	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	1	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	1	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	1	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	2	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	2	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	2	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	5	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	5	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	5	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	7	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	7	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD21	8	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD22	8	0.59
(1,996)	1:69:A:LEU:HB2	1:69:A:LEU:HD23	8	0.59
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	3	0.59
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	3	0.59
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB1	5	0.59
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB2	5	0.59
(1,775)	1:57:A:ARG:HB3	1:74:A:ALA:HB3	5	0.59
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	10	0.59
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	10	0.59
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	10	0.59
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	10	0.59
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	10	0.59
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	10	0.59
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	8	0.59
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	10	0.59
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	10	0.59
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	9	0.59
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	9	0.59
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	9	0.59
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	9	0.59
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	9	0.59
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	9	0.59
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG2	2	0.59
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG3	2	0.59
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	9	0.59
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	9	0.59
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	9	0.59
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	5	0.59
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	9	0.59
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	9	0.59
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	7	0.59
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	7	0.59
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	7	0.59
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	1	0.58
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	10	0.58
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	2	0.58
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	8	0.58
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	8	0.58
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	8	0.58
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	8	0.58
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	1	0.58
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	4	0.58
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	4	0.58
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	4	0.58
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	4	0.58
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	4	0.58
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	4	0.58
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	9	0.58
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	8	0.58
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	7	0.58
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	7	0.58
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	4	0.58
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	4	0.58
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	4	0.58
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	8	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG11	4	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG12	4	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG13	4	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG21	4	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG22	4	0.58
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG23	4	0.58
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	4	0.58
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	8	0.57
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	8	0.57
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	10	0.57
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	10	0.57
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	10	0.57
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	9	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	10	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	10	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	10	0.57
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	10	0.57
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	9	0.57
(1,592)	1:46:A:TYR:HB2	1:66:A:PHE:HE2	9	0.57
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:43:A:ALA:HB1	1:69:A:LEU:HG	7	0.57
(1,536)	1:43:A:ALA:HB2	1:69:A:LEU:HG	7	0.57
(1,536)	1:43:A:ALA:HB3	1:69:A:LEU:HG	7	0.57
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	1	0.57
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	1	0.57
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	1	0.57
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	4	0.57
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	8	0.57
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	8	0.57
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	7	0.57
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	8	0.57
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	8	0.57
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	7	0.57
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	9	0.56
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	1	0.56
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	9	0.56
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	9	0.56
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD2	9	0.56
(1,707)	1:52:A:ARG:HA	1:52:A:ARG:HD3	9	0.56
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	2	0.56
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	2	0.56
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	10	0.56
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB2	8	0.56
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB2	8	0.56
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB2	8	0.56
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB3	8	0.56
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB3	8	0.56
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB3	8	0.56
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	5	0.56
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	5	0.56
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	5	0.56
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	5	0.56
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	5	0.56
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	5	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	8	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	8	0.56
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	8	0.56
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	8	0.56
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	10	0.56
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	10	0.56
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	10	0.56
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	10	0.56
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	10	0.56
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	10	0.56
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	10	0.56
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	10	0.56
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	10	0.56
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	3	0.56
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	3	0.56
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	3	0.56
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	5	0.56
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	9	0.56
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	9	0.56
(1,19)	1:3:A:MET:HB2	1:5:A:PHE:HE1	2	0.56
(1,19)	1:3:A:MET:HB3	1:5:A:PHE:HE1	2	0.56
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	1	0.55
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	6	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG11	8	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG12	8	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG13	8	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG21	8	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG22	8	0.55
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG23	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG11	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG12	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG13	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG21	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG22	8	0.55
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG23	8	0.55
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	6	0.55
(1,882)	1:62:A:LEU:HB2	1:66:A:PHE:HD2	2	0.55
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	8	0.55
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	8	0.55
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	8	0.55
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD2	6	0.55
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD3	6	0.55
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	1	0.55
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	2	0.55
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	2	0.55
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	2	0.55
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	2	0.55
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	2	0.55
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	2	0.55
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	3	0.55
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	6	0.55
(1,343)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	5	0.55
(1,343)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	5	0.55
(1,343)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	5	0.55
(1,343)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	5	0.55
(1,343)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	5	0.55
(1,343)	1:24:A:VAL:HG21	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG21	1:32:A:ALA:HB2	5	0.55
(1,343)	1:24:A:VAL:HG21	1:32:A:ALA:HB3	5	0.55
(1,343)	1:24:A:VAL:HG22	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG22	1:32:A:ALA:HB2	5	0.55
(1,343)	1:24:A:VAL:HG22	1:32:A:ALA:HB3	5	0.55
(1,343)	1:24:A:VAL:HG23	1:32:A:ALA:HB1	5	0.55
(1,343)	1:24:A:VAL:HG23	1:32:A:ALA:HB2	5	0.55
(1,343)	1:24:A:VAL:HG23	1:32:A:ALA:HB3	5	0.55
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	8	0.55
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	3	0.55
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	3	0.55
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	3	0.55
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB1	8	0.55
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB2	8	0.55
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB3	8	0.55
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	2	0.54
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB1	3	0.54
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB2	3	0.54
(1,785)	1:58:A:VAL:H	1:74:A:ALA:HB3	3	0.54
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD2	4	0.54
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD3	4	0.54
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	5	0.54
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	5	0.54
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	5	0.54
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	5	0.54
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	5	0.54
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	5	0.54
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	5	0.54
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	9	0.54
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	3	0.54
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	3	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG11	4	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG12	4	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG13	4	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG21	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG22	4	0.54
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG23	4	0.54
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	7	0.54
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	7	0.54
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	7	0.54
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	7	0.54
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	7	0.54
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	7	0.54
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	1	0.54
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	1	0.54
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	1	0.54
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	1	0.54
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	1	0.54
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	1	0.54
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	10	0.54
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	10	0.54
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	3	0.54
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	3	0.54
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	3	0.54
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	2	0.53
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	2	0.53
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	2	0.53
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	2	0.53
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	2	0.53
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	2	0.53
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	8	0.53
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	2	0.53
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	4	0.53
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	5	0.53
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	5	0.53
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	5	0.53
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	5	0.53
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	5	0.53
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	5	0.53
(1,595)	1:46:A:TYR:HB3	1:46:A:TYR:HE1	4	0.53
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	1	0.53
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	9	0.53
(1,387)	1:27:A:VAL:HG11	1:50:A:VAL:HB	5	0.53
(1,387)	1:27:A:VAL:HG12	1:50:A:VAL:HB	5	0.53
(1,387)	1:27:A:VAL:HG13	1:50:A:VAL:HB	5	0.53
(1,387)	1:27:A:VAL:HG21	1:50:A:VAL:HB	5	0.53
(1,387)	1:27:A:VAL:HG22	1:50:A:VAL:HB	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:27:A:VAL:HG23	1:50:A:VAL:HB	5	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG11	3	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG12	3	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG13	3	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG21	3	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG22	3	0.53
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG23	3	0.53
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	3	0.53
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	3	0.53
(1,160)	1:16:A:ALA:HA	1:19:A:ALA:H	1	0.53
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	6	0.53
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	2	0.53
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	2	0.53
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	2	0.53
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	9	0.53
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	4	0.52
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	4	0.52
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	4	0.52
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	10	0.52
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	10	0.52
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	10	0.52
(1,771)	1:57:A:ARG:HB2	1:74:A:ALA:H	10	0.52
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	3	0.52
(1,595)	1:46:A:TYR:HB3	1:46:A:TYR:HE1	5	0.52
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	6	0.52
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	6	0.52
(1,101)	1:12:A:THR:HA	1:12:A:THR:HB	4	0.52
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	3	0.51
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	3	0.51
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	3	0.51
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	3	0.51
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	3	0.51
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	3	0.51
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	4	0.51
(1,796)	1:58:A:VAL:HG11	1:60:A:VAL:HA	4	0.51
(1,796)	1:58:A:VAL:HG12	1:60:A:VAL:HA	4	0.51
(1,796)	1:58:A:VAL:HG13	1:60:A:VAL:HA	4	0.51
(1,796)	1:58:A:VAL:HG21	1:60:A:VAL:HA	4	0.51
(1,796)	1:58:A:VAL:HG22	1:60:A:VAL:HA	4	0.51
(1,796)	1:58:A:VAL:HG23	1:60:A:VAL:HA	4	0.51
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	5	0.51
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	5	0.51
(1,603)	1:46:A:TYR:HB3	1:66:A:PHE:HZ	3	0.51
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	2	0.51
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	4	0.51
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB2	5	0.51
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB3	5	0.51
(1,101)	1:12:A:THR:HA	1:12:A:THR:HB	3	0.51
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	4	0.5
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	8	0.5
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	8	0.5
(1,693)	1:51:A:THR:HG21	1:54:A:ASP:H	8	0.5
(1,693)	1:51:A:THR:HG22	1:54:A:ASP:H	8	0.5
(1,693)	1:51:A:THR:HG23	1:54:A:ASP:H	8	0.5
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD2	9	0.5
(1,684)	1:51:A:THR:H	1:57:A:ARG:HD3	9	0.5
(1,595)	1:46:A:TYR:HB3	1:46:A:TYR:HE1	10	0.5
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	2	0.5
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	1	0.5
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	1	0.5
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	1	0.5
(1,491)	1:37:A:THR:HG21	1:46:A:TYR:HD1	6	0.5
(1,491)	1:37:A:THR:HG22	1:46:A:TYR:HD1	6	0.5
(1,491)	1:37:A:THR:HG23	1:46:A:TYR:HD1	6	0.5
(1,422)	1:32:A:ALA:HB1	1:49:A:LEU:HG	10	0.5
(1,422)	1:32:A:ALA:HB2	1:49:A:LEU:HG	10	0.5
(1,422)	1:32:A:ALA:HB3	1:49:A:LEU:HG	10	0.5
(1,198)	1:18:A:ARG:HA	1:66:A:PHE:HZ	10	0.5
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	1	0.5
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	2	0.5
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	10	0.5
(1,148)	1:15:A:ASP:HB2	1:66:A:PHE:HE1	1	0.5
(1,148)	1:15:A:ASP:HB3	1:66:A:PHE:HE1	1	0.5
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	2	0.49
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	10	0.49
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	10	0.49
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	7	0.49
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	7	0.49
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	7	0.49
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	7	0.49
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	7	0.49
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	7	0.49
(1,920)	1:63:A:ASP:HB2	1:65:A:ASP:H	10	0.49
(1,918)	1:63:A:ASP:HB2	1:64:A:ARG:H	3	0.49
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	6	0.49
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	6	0.49
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	6	0.49
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	6	0.49
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	6	0.49
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	6	0.49
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	3	0.49
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	3	0.49
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	3	0.49
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	3	0.49
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	3	0.49
(1,602)	1:46:A:TYR:HB3	1:66:A:PHE:HE1	2	0.49
(1,593)	1:46:A:TYR:HB2	1:66:A:PHE:HZ	3	0.49
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	8	0.49
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	8	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	7	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	7	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	7	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	7	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	7	0.49
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	7	0.49
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	7	0.49
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	7	0.49
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	8	0.49
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	8	0.49
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	8	0.49
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	8	0.49
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	8	0.49
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	8	0.49
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	10	0.49
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB2	6	0.49
(1,284)	1:22:A:ALA:HA	1:25:A:GLN:HB3	6	0.49
(1,146)	1:15:A:ASP:HB2	1:37:A:THR:H	10	0.49
(1,146)	1:15:A:ASP:HB3	1:37:A:THR:H	10	0.49
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	5	0.49
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	4	0.49
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	9	0.49
(1,9)	1:3:A:MET:HG2	1:5:A:PHE:HB2	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:59:A:GLU:HG2	1:74:A:ALA:HA	2	0.48
(1,814)	1:59:A:GLU:HG3	1:74:A:ALA:HA	2	0.48
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	4	0.48
(1,741)	1:54:A:ASP:H	1:56:A:THR:HB	3	0.48
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	9	0.48
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	9	0.48
(1,693)	1:51:A:THR:HG21	1:54:A:ASP:H	10	0.48
(1,693)	1:51:A:THR:HG22	1:54:A:ASP:H	10	0.48
(1,693)	1:51:A:THR:HG23	1:54:A:ASP:H	10	0.48
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	3	0.48
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	3	0.48
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	3	0.48
(1,202)	1:18:A:ARG:HB2	1:66:A:PHE:HE1	5	0.48
(1,202)	1:18:A:ARG:HB2	1:66:A:PHE:HE1	10	0.48
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	7	0.48
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	7	0.48
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	5	0.47
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	9	0.47
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	9	0.47
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	9	0.47
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	9	0.47
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	9	0.47
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	9	0.47
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	9	0.47
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	9	0.47
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	9	0.47
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD21	8	0.47
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD22	8	0.47
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD23	8	0.47
(1,584)	1:46:A:TYR:HA	1:62:A:LEU:HB3	8	0.47
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG11	8	0.47
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG12	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG13	8	0.47
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG21	8	0.47
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG22	8	0.47
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG23	8	0.47
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	6	0.47
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	6	0.47
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	6	0.47
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	6	0.47
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	6	0.47
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	6	0.47
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	8	0.47
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	3	0.47
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	3	0.47
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	3	0.47
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	3	0.47
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	3	0.47
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	3	0.47
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB1	2	0.47
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB2	2	0.47
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB3	2	0.47
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	7	0.47
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	7	0.47
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	7	0.47
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	8	0.47
(1,87)	1:10:A:GLU:HA	1:11:A:VAL:H	6	0.47
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	3	0.46
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	3	0.46
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	8	0.46
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	10	0.46
(1,811)	1:59:A:GLU:HG3	1:74:A:ALA:HA	9	0.46
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	6	0.46
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	6	0.46
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	6	0.46
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	6	0.46
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	6	0.46
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	6	0.46
(1,578)	1:46:A:TYR:H	1:62:A:LEU:HG	4	0.46
(1,573)	1:46:A:TYR:H	1:46:A:TYR:HD2	10	0.46
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	1	0.46
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	6	0.46
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	6	0.46
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	6	0.46
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	6	0.46
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	6	0.46
(1,311)	1:23:A:ALA:HB1	1:51:A:THR:H	7	0.46
(1,311)	1:23:A:ALA:HB2	1:51:A:THR:H	7	0.46
(1,311)	1:23:A:ALA:HB3	1:51:A:THR:H	7	0.46
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	1	0.46
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	1	0.46
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	1	0.46
(1,210)	1:18:A:ARG:HG3	1:19:A:ALA:H	8	0.46
(1,206)	1:18:A:ARG:HB3	1:66:A:PHE:HE1	1	0.46
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	2	0.46
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	7	0.46
(1,109)	1:13:A:GLY:HA2	1:14:A:PRO:HG2	8	0.46
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	2	0.45
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	10	0.45
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	10	0.45
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	3	0.45
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	3	0.45
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	3	0.45
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	6	0.45
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	5	0.45
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	10	0.45
(1,820)	1:60:A:VAL:HA	1:61:A:HIS:HD2	8	0.45
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	3	0.45
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	3	0.45
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	3	0.45
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	9	0.45
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	9	0.45
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	9	0.45
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	7	0.45
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	9	0.45
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	9	0.45
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	9	0.45
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	9	0.45
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	9	0.45
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	5	0.45
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	7	0.45
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	7	0.45
(1,557)	1:44:A:ALA:HB1	1:62:A:LEU:H	7	0.45
(1,557)	1:44:A:ALA:HB2	1:62:A:LEU:H	7	0.45
(1,557)	1:44:A:ALA:HB3	1:62:A:LEU:H	7	0.45
(1,553)	1:44:A:ALA:HB1	1:46:A:TYR:H	8	0.45
(1,553)	1:44:A:ALA:HB2	1:46:A:TYR:H	8	0.45
(1,553)	1:44:A:ALA:HB3	1:46:A:TYR:H	8	0.45
(1,551)	1:44:A:ALA:HA	1:69:A:LEU:HG	4	0.45
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	6	0.45
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	6	0.45
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	6	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG11	8	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG12	8	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG13	8	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG21	8	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG22	8	0.45
(1,407)	1:31:A:THR:H	1:50:A:VAL:HG23	8	0.45
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	4	0.45
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	6	0.45
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD2	7	0.45
(1,132)	1:15:A:ASP:HA	1:18:A:ARG:HD3	7	0.45
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	8	0.45
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	5	0.45
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	3	0.44
(1,591)	1:46:A:TYR:HB2	1:66:A:PHE:HA	10	0.44
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	7	0.44
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	7	0.44
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	7	0.44
(1,371)	1:27:A:VAL:HA	1:28:A:PRO:HB3	6	0.44
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	7	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG11	3	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG12	3	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG13	3	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG21	3	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG22	3	0.44
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG23	3	0.44
(1,248)	1:20:A:ARG:HB2	1:35:A:VAL:H	10	0.44
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	6	0.44
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB1	2	0.44
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB2	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:15:A:ASP:HB3	1:19:A:ALA:HB3	2	0.44
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	8	0.44
(1,61)	1:6:A:ASP:H	1:7:A:GLY:H	5	0.44
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	2	0.44
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	9	0.43
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	9	0.43
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	9	0.43
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	9	0.43
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	9	0.43
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	9	0.43
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	3	0.43
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	4	0.43
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	5	0.43
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	9	0.43
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	2	0.43
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	2	0.43
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	2	0.43
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	2	0.43
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	2	0.43
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	2	0.43
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	2	0.43
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	1	0.43
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	1	0.43
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	10	0.43
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	6	0.43
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	6	0.43
(1,371)	1:27:A:VAL:HA	1:28:A:PRO:HB3	7	0.43
(1,261)	1:20:A:ARG:HG3	1:33:A:GLY:H	9	0.43
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	4	0.43
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	4	0.43
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	4	0.43
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	3	0.43
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	3	0.43
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	3	0.43
(1,209)	1:18:A:ARG:HG2	1:20:A:ARG:H	9	0.43
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	6	0.43
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	6	0.43
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	6	0.43
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	7	0.43
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	2	0.43
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	9	0.43
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	3	0.43
(1,920)	1:63:A:ASP:HB2	1:65:A:ASP:H	4	0.42
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	4	0.42
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	3	0.42
(1,721)	1:52:A:ARG:HG2	1:56:A:THR:H	1	0.42
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	9	0.42
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	9	0.42
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	9	0.42
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	9	0.42
(1,387)	1:27:A:VAL:HG11	1:50:A:VAL:HB	10	0.42
(1,387)	1:27:A:VAL:HG12	1:50:A:VAL:HB	10	0.42
(1,387)	1:27:A:VAL:HG13	1:50:A:VAL:HB	10	0.42
(1,387)	1:27:A:VAL:HG21	1:50:A:VAL:HB	10	0.42
(1,387)	1:27:A:VAL:HG22	1:50:A:VAL:HB	10	0.42
(1,387)	1:27:A:VAL:HG23	1:50:A:VAL:HB	10	0.42
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	4	0.42
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	1	0.42
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	1	0.42
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	1	0.42
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	1	0.42
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	1	0.42
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	8	0.42
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	8	0.42
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	8	0.42
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	8	0.42
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	8	0.42
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	8	0.42
(1,241)	1:20:A:ARG:HA	1:23:A:ALA:HA	4	0.42
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	8	0.42
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	8	0.42
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	8	0.42
(1,207)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	8	0.42
(1,207)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	8	0.42
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	5	0.42
(1,160)	1:16:A:ALA:HA	1:19:A:ALA:H	3	0.42
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	10	0.41
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	10	0.41
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	6	0.41
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	10	0.41
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD11	1:57:A:ARG:HB3	3	0.41
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD12	1:57:A:ARG:HB3	3	0.41
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD13	1:57:A:ARG:HB3	3	0.41
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD21	1:57:A:ARG:HB3	3	0.41
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD22	1:57:A:ARG:HB3	3	0.41
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB2	3	0.41
(1,661)	1:49:A:LEU:HD23	1:57:A:ARG:HB3	3	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	8	0.41
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	8	0.41
(1,582)	1:46:A:TYR:HA	1:46:A:TYR:HE1	10	0.41
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	6	0.41
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	6	0.41
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	6	0.41
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	3	0.41
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	3	0.41
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	3	0.41
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	3	0.41
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	3	0.41
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	3	0.41
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	5	0.41
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	5	0.41
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	5	0.41
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	5	0.41
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	5	0.41
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	5	0.41
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	5	0.41
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	5	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	9	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	9	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	9	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	9	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	9	0.41
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	9	0.41
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	10	0.41
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	3	0.41
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	3	0.41
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	3	0.41
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB2	8	0.41
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB3	8	0.41
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	7	0.41
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	6	0.4
(1,721)	1:52:A:ARG:HG2	1:56:A:THR:H	10	0.4
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	8	0.4
(1,535)	1:43:A:ALA:HB1	1:63:A:ASP:HB2	4	0.4
(1,535)	1:43:A:ALA:HB2	1:63:A:ASP:HB2	4	0.4
(1,535)	1:43:A:ALA:HB3	1:63:A:ASP:HB2	4	0.4
(1,391)	1:27:A:VAL:HG11	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG11	1:52:A:ARG:HG3	2	0.4
(1,391)	1:27:A:VAL:HG12	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG12	1:52:A:ARG:HG3	2	0.4
(1,391)	1:27:A:VAL:HG13	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG13	1:52:A:ARG:HG3	2	0.4
(1,391)	1:27:A:VAL:HG21	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG21	1:52:A:ARG:HG3	2	0.4
(1,391)	1:27:A:VAL:HG22	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG22	1:52:A:ARG:HG3	2	0.4
(1,391)	1:27:A:VAL:HG23	1:52:A:ARG:HG2	2	0.4
(1,391)	1:27:A:VAL:HG23	1:52:A:ARG:HG3	2	0.4
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	9	0.4
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	9	0.4
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	9	0.4
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	9	0.4
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	9	0.4
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	9	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	9	0.4
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	9	0.4
(1,217)	1:19:A:ALA:H	1:66:A:PHE:HE1	9	0.4
(1,180)	1:17:A:ASP:HA	1:20:A:ARG:HB3	10	0.4
(1,119)	1:14:A:PRO:HD2	1:15:A:ASP:H	8	0.4
(1,119)	1:14:A:PRO:HD3	1:15:A:ASP:H	8	0.4
(1,59)	1:5:A:PHE:HE2	1:66:A:PHE:H	3	0.4
(1,32)	1:5:A:PHE:H	1:66:A:PHE:HD1	9	0.4
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	2	0.39
(1,974)	1:67:A:ARG:HG2	1:68:A:VAL:HB	8	0.39
(1,974)	1:67:A:ARG:HG3	1:68:A:VAL:HB	8	0.39
(1,954)	1:65:A:ASP:HB2	1:67:A:ARG:HA	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	1	0.39
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	1	0.39
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	1	0.39
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	1	0.39
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	10	0.39
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	10	0.39
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	10	0.39
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	10	0.39
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	10	0.39
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	10	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	9	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	9	0.39
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	9	0.39
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	9	0.39
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	9	0.39
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	9	0.39
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	9	0.39
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	6	0.39
(1,547)	1:44:A:ALA:HA	1:63:A:ASP:H	2	0.39
(1,513)	1:38:A:GLU:HG2	1:46:A:TYR:HA	5	0.39
(1,513)	1:38:A:GLU:HG3	1:46:A:TYR:HA	5	0.39
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	6	0.39
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	6	0.39
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	6	0.39
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	10	0.39
(1,149)	1:15:A:ASP:HB2	1:66:A:PHE:HZ	5	0.39
(1,149)	1:15:A:ASP:HB3	1:66:A:PHE:HZ	5	0.39
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	7	0.39
(1,45)	1:5:A:PHE:HB3	1:66:A:PHE:HD1	3	0.39
(1,40)	1:5:A:PHE:HB2	1:66:A:PHE:HD1	3	0.39
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	7	0.39
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	3	0.38
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	3	0.38
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	3	0.38
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	5	0.38
(1,802)	1:59:A:GLU:H	1:74:A:ALA:HA	9	0.38
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	7	0.38
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	3	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	1	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	1	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	1	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	1	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	1	0.38
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	1	0.38
(1,273)	1:21:A:ALA:H	1:24:A:VAL:H	5	0.38
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	7	0.38
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	7	0.38
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	7	0.38
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	8	0.38
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	8	0.38
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	8	0.38
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	10	0.37
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	10	0.37
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	6	0.37
(1,937)	1:64:A:ARG:HA	1:64:A:ARG:HG2	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	7	0.37
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	7	0.37
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	7	0.37
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	4	0.37
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	6	0.37
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	6	0.37
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	6	0.37
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	5	0.37
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	10	0.37
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	10	0.37
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	10	0.37
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	10	0.37
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	10	0.37
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	10	0.37
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	1	0.37
(1,512)	1:38:A:GLU:HG2	1:45:A:ALA:HA	1	0.37
(1,512)	1:38:A:GLU:HG3	1:45:A:ALA:HA	1	0.37
(1,498)	1:38:A:GLU:H	1:46:A:TYR:HB3	9	0.37
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	2	0.37
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	2	0.37
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	2	0.37
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	2	0.37
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	2	0.37
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	2	0.37
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	10	0.37
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	7	0.37
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	7	0.37
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	7	0.37
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	7	0.37
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	7	0.37
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	7	0.37
(1,212)	1:18:A:ARG:HD2	1:66:A:PHE:HE1	6	0.37
(1,212)	1:18:A:ARG:HD3	1:66:A:PHE:HE1	6	0.37
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB2	4	0.37
(1,131)	1:15:A:ASP:HA	1:18:A:ARG:HB3	4	0.37
(2,4)	1:31:A:THR:O	1:51:A:THR:H	6	0.36
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	5	0.36
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	5	0.36
(1,843)	1:61:A:HIS:HA	1:69:A:LEU:HB2	7	0.36
(1,814)	1:59:A:GLU:HG2	1:74:A:ALA:HA	8	0.36
(1,814)	1:59:A:GLU:HG3	1:74:A:ALA:HA	8	0.36
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	9	0.36
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	7	0.36
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	4	0.36
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	4	0.36
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	4	0.36
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	5	0.36
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	5	0.36
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	5	0.36
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	5	0.36
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	5	0.36
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	5	0.36
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	5	0.36
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	5	0.36
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	5	0.36
(1,61)	1:6:A:ASP:H	1:7:A:GLY:H	3	0.36
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	4	0.36
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	4	0.36
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	9	0.35
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	6	0.35
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	6	0.35
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	10	0.35
(1,850)	1:61:A:HIS:HB2	1:69:A:LEU:HG	10	0.35
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	9	0.35
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	9	0.35
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	9	0.35
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	9	0.35
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	9	0.35
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	9	0.35
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	8	0.35
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	4	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	6	0.35
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	6	0.35
(1,550)	1:44:A:ALA:HA	1:69:A:LEU:HB2	5	0.35
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	1	0.35
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	1	0.35
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	1	0.35
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	1	0.35
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	1	0.35
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	1	0.35
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	8	0.35
(1,330)	1:24:A:VAL:HG11	1:32:A:ALA:H	9	0.35
(1,330)	1:24:A:VAL:HG12	1:32:A:ALA:H	9	0.35
(1,330)	1:24:A:VAL:HG13	1:32:A:ALA:H	9	0.35
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	10	0.35
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	4	0.35
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	8	0.35
(1,263)	1:20:A:ARG:HG3	1:34:A:GLU:H	5	0.35
(1,154)	1:16:A:ALA:H	1:18:A:ARG:HG2	9	0.35
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	4	0.35
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:61:A:HIS:HB3	1:68:A:VAL:HA	5	0.34
(1,847)	1:61:A:HIS:HB2	1:68:A:VAL:HA	8	0.34
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	5	0.34
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	1	0.34
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	4	0.34
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	4	0.34
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	4	0.34
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	4	0.34
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	4	0.34
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	4	0.34
(1,658)	1:49:A:LEU:HD11	1:57:A:ARG:HA	2	0.34
(1,658)	1:49:A:LEU:HD12	1:57:A:ARG:HA	2	0.34
(1,658)	1:49:A:LEU:HD13	1:57:A:ARG:HA	2	0.34
(1,637)	1:48:A:VAL:HG11	1:49:A:LEU:HA	2	0.34
(1,637)	1:48:A:VAL:HG12	1:49:A:LEU:HA	2	0.34
(1,637)	1:48:A:VAL:HG13	1:49:A:LEU:HA	2	0.34
(1,637)	1:48:A:VAL:HG21	1:49:A:LEU:HA	2	0.34
(1,637)	1:48:A:VAL:HG22	1:49:A:LEU:HA	2	0.34
(1,637)	1:48:A:VAL:HG23	1:49:A:LEU:HA	2	0.34
(1,617)	1:47:A:GLY:H	1:62:A:LEU:HB2	8	0.34
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB2	6	0.34
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB2	6	0.34
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB2	6	0.34
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB3	6	0.34
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB3	6	0.34
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB3	6	0.34
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB1	4	0.34
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB2	4	0.34
(1,510)	1:38:A:GLU:HG2	1:44:A:ALA:HB3	4	0.34
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB1	4	0.34
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB2	4	0.34
(1,510)	1:38:A:GLU:HG3	1:44:A:ALA:HB3	4	0.34
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	1	0.34
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	1	0.34
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	1	0.34
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	1	0.34
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	1	0.34
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	1	0.34
(1,302)	1:23:A:ALA:HA	1:50:A:VAL:HB	1	0.34
(1,248)	1:20:A:ARG:HB2	1:35:A:VAL:H	4	0.34
(1,96)	1:11:A:VAL:HB	1:12:A:THR:H	2	0.34
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	9	0.34
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	2	0.33
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	2	0.33
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	2	0.33
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	5	0.33
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	5	0.33
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	5	0.33
(1,723)	1:52:A:ARG:HG3	1:56:A:THR:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	9	0.33
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	9	0.33
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	9	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG11	1:60:A:VAL:HG23	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG12	1:60:A:VAL:HG23	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG13	1:60:A:VAL:HG23	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG21	1:60:A:VAL:HG23	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG22	1:60:A:VAL:HG23	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG11	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG12	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG13	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG21	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG22	2	0.33
(1,641)	1:48:A:VAL:HG23	1:60:A:VAL:HG23	2	0.33
(1,591)	1:46:A:TYR:HB2	1:66:A:PHE:HA	8	0.33
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	9	0.33
(1,574)	1:46:A:TYR:H	1:46:A:TYR:HE2	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG11	1	0.33
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG12	1	0.33
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG13	1	0.33
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG21	1	0.33
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG22	1	0.33
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG23	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG11	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG12	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG13	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG21	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG22	1	0.33
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG23	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG11	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG12	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG13	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG21	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG22	1	0.33
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG23	1	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	3	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	3	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	3	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	3	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	3	0.33
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	3	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	8	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	8	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	8	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	8	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	8	0.33
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	8	0.33
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	2	0.33
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	2	0.33
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	2	0.33
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	6	0.33
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	2	0.33
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	1	0.32
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	7	0.32
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	7	0.32
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	7	0.32
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	7	0.32
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	7	0.32
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	3	0.32
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	3	0.32
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB2	8	0.32
(1,609)	1:46:A:TYR:HE2	1:62:A:LEU:HB3	8	0.32
(1,557)	1:44:A:ALA:HB1	1:62:A:LEU:H	5	0.32
(1,557)	1:44:A:ALA:HB2	1:62:A:LEU:H	5	0.32
(1,557)	1:44:A:ALA:HB3	1:62:A:LEU:H	5	0.32
(1,554)	1:44:A:ALA:HB1	1:61:A:HIS:HA	6	0.32
(1,554)	1:44:A:ALA:HB2	1:61:A:HIS:HA	6	0.32
(1,554)	1:44:A:ALA:HB3	1:61:A:HIS:HA	6	0.32
(1,333)	1:24:A:VAL:HG21	1:32:A:ALA:H	1	0.32
(1,333)	1:24:A:VAL:HG22	1:32:A:ALA:H	1	0.32
(1,333)	1:24:A:VAL:HG23	1:32:A:ALA:H	1	0.32
(1,263)	1:20:A:ARG:HG3	1:34:A:GLU:H	3	0.32
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	4	0.32
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	4	0.32
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	4	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG11	6	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG12	6	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG13	6	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG21	6	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG22	6	0.32
(1,245)	1:20:A:ARG:HA	1:48:A:VAL:HG23	6	0.32
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	10	0.32
(1,96)	1:11:A:VAL:HB	1:12:A:THR:H	8	0.32
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	9	0.32
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	3	0.31
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	9	0.31
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	4	0.31
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	4	0.31
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	4	0.31
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	10	0.31
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	10	0.31
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	10	0.31
(1,509)	1:38:A:GLU:HG2	1:44:A:ALA:HA	8	0.31
(1,509)	1:38:A:GLU:HG3	1:44:A:ALA:HA	8	0.31
(1,483)	1:37:A:THR:HA	1:46:A:TYR:HE1	9	0.31
(1,380)	1:27:A:VAL:HG11	1:31:A:THR:HB	9	0.31
(1,380)	1:27:A:VAL:HG12	1:31:A:THR:HB	9	0.31
(1,380)	1:27:A:VAL:HG13	1:31:A:THR:HB	9	0.31
(1,341)	1:24:A:VAL:HG11	1:31:A:THR:H	8	0.31
(1,341)	1:24:A:VAL:HG12	1:31:A:THR:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:24:A:VAL:HG13	1:31:A:THR:H	8	0.31
(1,341)	1:24:A:VAL:HG21	1:31:A:THR:H	8	0.31
(1,341)	1:24:A:VAL:HG22	1:31:A:THR:H	8	0.31
(1,341)	1:24:A:VAL:HG23	1:31:A:THR:H	8	0.31
(1,311)	1:23:A:ALA:HB1	1:51:A:THR:H	1	0.31
(1,311)	1:23:A:ALA:HB2	1:51:A:THR:H	1	0.31
(1,311)	1:23:A:ALA:HB3	1:51:A:THR:H	1	0.31
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	9	0.31
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	3	0.31
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	3	0.31
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	3	0.31
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	10	0.31
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	10	0.31
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	10	0.31
(1,118)	1:14:A:PRO:HG2	1:17:A:ASP:H	1	0.31
(1,115)	1:14:A:PRO:HA	1:17:A:ASP:H	8	0.31
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	3	0.3
(1,974)	1:67:A:ARG:HG2	1:68:A:VAL:HB	3	0.3
(1,974)	1:67:A:ARG:HG3	1:68:A:VAL:HB	3	0.3
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	7	0.3
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	8	0.3
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB1	2	0.3
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB2	2	0.3
(1,764)	1:57:A:ARG:H	1:74:A:ALA:HB3	2	0.3
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	3	0.3
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	3	0.3
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	3	0.3
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	6	0.3
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	4	0.3
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	3	0.3
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	3	0.3
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	3	0.3
(1,487)	1:37:A:THR:HB	1:46:A:TYR:HD1	9	0.3
(1,354)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	10	0.3
(1,354)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	10	0.3
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	2	0.3
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	2	0.3
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	2	0.3
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	2	0.3
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	2	0.3
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	2	0.3
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	6	0.3
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	6	0.3
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	6	0.3
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	6	0.3
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	6	0.3
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	6	0.3
(1,160)	1:16:A:ALA:HA	1:19:A:ALA:H	7	0.3
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB1	8	0.3
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB2	8	0.3
(1,136)	1:15:A:ASP:HB2	1:19:A:ALA:HB3	8	0.3
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	6	0.3
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	8	0.3
(1,117)	1:14:A:PRO:HG2	1:16:A:ALA:H	5	0.3
(1,99)	1:12:A:THR:H	1:12:A:THR:HG21	4	0.3
(1,99)	1:12:A:THR:H	1:12:A:THR:HG22	4	0.3
(1,99)	1:12:A:THR:H	1:12:A:THR:HG23	4	0.3
(1,96)	1:11:A:VAL:HB	1:12:A:THR:H	7	0.3
(1,96)	1:11:A:VAL:HB	1:12:A:THR:H	9	0.3
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG21	7	0.3
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG22	7	0.3
(1,95)	1:11:A:VAL:HA	1:12:A:THR:HG23	7	0.3
(1,87)	1:10:A:GLU:HA	1:11:A:VAL:H	4	0.3
(1,85)	1:10:A:GLU:H	1:10:A:GLU:HG2	5	0.3
(1,85)	1:10:A:GLU:H	1:10:A:GLU:HG3	5	0.3
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	10	0.3
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	4	0.29
(1,946)	1:64:A:ARG:HG2	1:66:A:PHE:H	1	0.29
(1,946)	1:64:A:ARG:HG3	1:66:A:PHE:H	1	0.29
(1,937)	1:64:A:ARG:HA	1:64:A:ARG:HG2	2	0.29
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	5	0.29
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	5	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	5	0.29
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	5	0.29
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	5	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	5	0.29
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	8	0.29
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	8	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	8	0.29
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	8	0.29
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	8	0.29
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	8	0.29
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	8	0.29
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	8	0.29
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	7	0.29
(1,823)	1:60:A:VAL:HA	1:72:A:GLU:H	1	0.29
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB1	6	0.29
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB2	6	0.29
(1,790)	1:58:A:VAL:HA	1:74:A:ALA:HB3	6	0.29
(1,771)	1:57:A:ARG:HB2	1:74:A:ALA:H	8	0.29
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	3	0.29
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	3	0.29
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	3	0.29
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	3	0.29
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	3	0.29
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	3	0.29
(1,655)	1:49:A:LEU:HB3	1:49:A:LEU:HG	8	0.29
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	5	0.29
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	5	0.29
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	5	0.29
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	5	0.29
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	5	0.29
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	5	0.29
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	6	0.29
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	6	0.29
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	6	0.29
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	6	0.29
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	6	0.29
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	6	0.29
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	6	0.29
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	6	0.29
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	6	0.29
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	7	0.29
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	4	0.29
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	1	0.29
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	1	0.29
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	1	0.29
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	2	0.29
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	2	0.29
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	2	0.29
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	9	0.29
(1,117)	1:14:A:PRO:HG2	1:16:A:ALA:H	2	0.29
(1,87)	1:10:A:GLU:HA	1:11:A:VAL:H	1	0.29
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	1	0.28
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	1	0.28
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	1	0.28
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	1	0.28
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	1	0.28
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	10	0.28
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	10	0.28
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	10	0.28
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	10	0.28
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	10	0.28
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	10	0.28
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	1	0.28
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	1	0.28
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	1	0.28
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	1	0.28
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	1	0.28
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	1	0.28
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	9	0.28
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	5	0.28
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	9	0.28
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	9	0.28
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	1	0.28
(1,802)	1:59:A:GLU:H	1:74:A:ALA:HA	8	0.28
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	7	0.28
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	7	0.28
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	7	0.28
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	7	0.28
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	3	0.28
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	5	0.28
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	6	0.28
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	6	0.28
(1,625)	1:47:A:GLY:HA3	1:62:A:LEU:H	2	0.28
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	5	0.28
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	5	0.28
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	5	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	10	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	10	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	10	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	10	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	10	0.28
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	10	0.28
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	10	0.28
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	10	0.28
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	10	0.28
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	10	0.28
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	10	0.28
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	10	0.28
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	10	0.28
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	10	0.28
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	10	0.28
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB1	6	0.28
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB2	6	0.28
(1,258)	1:20:A:ARG:HG2	1:32:A:ALA:HB3	6	0.28
(1,241)	1:20:A:ARG:HA	1:23:A:ALA:HA	7	0.28
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	6	0.28
(1,117)	1:14:A:PRO:HG2	1:16:A:ALA:H	9	0.28
(1,99)	1:12:A:THR:H	1:12:A:THR:HG21	3	0.28
(1,99)	1:12:A:THR:H	1:12:A:THR:HG22	3	0.28
(1,99)	1:12:A:THR:H	1:12:A:THR:HG23	3	0.28
(1,87)	1:10:A:GLU:HA	1:11:A:VAL:H	10	0.28
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB2	1	0.28
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB3	1	0.28
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	9	0.28
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	2	0.27
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	2	0.27
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	1	0.27
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	2	0.27
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	6	0.27
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	6	0.27
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	6	0.27
(1,721)	1:52:A:ARG:HG2	1:56:A:THR:H	8	0.27
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	1	0.27
(1,655)	1:49:A:LEU:HB3	1:49:A:LEU:HG	6	0.27
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	7	0.27
(1,556)	1:44:A:ALA:HB1	1:61:A:HIS:HD2	4	0.27
(1,556)	1:44:A:ALA:HB2	1:61:A:HIS:HD2	4	0.27
(1,556)	1:44:A:ALA:HB3	1:61:A:HIS:HD2	4	0.27
(1,553)	1:44:A:ALA:HB1	1:46:A:TYR:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:44:A:ALA:HB2	1:46:A:TYR:H	7	0.27
(1,553)	1:44:A:ALA:HB3	1:46:A:TYR:H	7	0.27
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	10	0.27
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	10	0.27
(1,511)	1:38:A:GLU:HG2	1:45:A:ALA:H	8	0.27
(1,511)	1:38:A:GLU:HG3	1:45:A:ALA:H	8	0.27
(1,506)	1:38:A:GLU:HB2	1:40:A:GLY:H	10	0.27
(1,506)	1:38:A:GLU:HB3	1:40:A:GLY:H	10	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG11	3	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG12	3	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG13	3	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG21	3	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG22	3	0.27
(1,417)	1:32:A:ALA:H	1:50:A:VAL:HG23	3	0.27
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	4	0.27
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	7	0.27
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	7	0.27
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	7	0.27
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	7	0.27
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	7	0.27
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	7	0.27
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD2	6	0.27
(1,374)	1:27:A:VAL:HA	1:52:A:ARG:HD3	6	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	5	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	5	0.27
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	5	0.27
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	5	0.27
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	5	0.27
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	2	0.27
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	5	0.27
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	5	0.27
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	5	0.27
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	6	0.27
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	6	0.27
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	6	0.27
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	10	0.27
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	1	0.27
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	5	0.27
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	10	0.27
(2,4)	1:31:A:THR:O	1:51:A:THR:H	8	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD11	4	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD12	4	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD13	4	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD21	4	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD22	4	0.26
(1,947)	1:64:A:ARG:HG2	1:69:A:LEU:HD23	4	0.26
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD11	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD12	4	0.26
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD13	4	0.26
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD21	4	0.26
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD22	4	0.26
(1,947)	1:64:A:ARG:HG3	1:69:A:LEU:HD23	4	0.26
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	2	0.26
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	3	0.26
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	10	0.26
(1,763)	1:57:A:ARG:H	1:74:A:ALA:H	10	0.26
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	1	0.26
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	9	0.26
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	9	0.26
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	9	0.26
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	9	0.26
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	9	0.26
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	9	0.26
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	3	0.26
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	3	0.26
(1,591)	1:46:A:TYR:HB2	1:66:A:PHE:HA	6	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG11	2	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG12	2	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG13	2	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG21	2	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG22	2	0.26
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG23	2	0.26
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG11	1:52:A:ARG:HD3	1	0.26
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG12	1:52:A:ARG:HD3	1	0.26
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG13	1:52:A:ARG:HD3	1	0.26
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG21	1:52:A:ARG:HD3	1	0.26
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG22	1:52:A:ARG:HD3	1	0.26
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD2	1	0.26
(1,390)	1:27:A:VAL:HG23	1:52:A:ARG:HD3	1	0.26
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	2	0.26
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	4	0.26
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	4	0.26
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	4	0.26
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	4	0.26
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	4	0.26
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	10	0.26
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	10	0.26
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	10	0.26
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	10	0.26
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	10	0.26
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	10	0.26
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	3	0.26
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB2	9	0.26
(1,48)	1:5:A:PHE:HB3	1:6:A:ASP:HB3	9	0.26
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB1	1	0.26
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB2	1	0.26
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB3	1	0.26
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB1	1	0.26
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB2	1	0.26
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB3	1	0.26
(2,6)	1:33:A:GLY:H	1:49:A:LEU:O	10	0.25
(2,3)	1:31:A:THR:O	1:51:A:THR:N	6	0.25
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	10	0.25
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB2	6	0.25
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB3	6	0.25
(1,954)	1:65:A:ASP:HB2	1:67:A:ARG:HA	4	0.25
(1,892)	1:62:A:LEU:HB3	1:68:A:VAL:HA	1	0.25
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	2	0.25
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	2	0.25
(1,777)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	2	0.25
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	5	0.25
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	5	0.25
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	5	0.25
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	5	0.25
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	5	0.25
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	5	0.25
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD2	1	0.25
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD3	1	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	2	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	2	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	2	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	2	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	2	0.25
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	2	0.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	2	0.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	2	0.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	2	0.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	2	0.25
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	2	0.25
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	2	0.25
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	9	0.25
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	9	0.25
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	9	0.25
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	9	0.25
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	9	0.25
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	9	0.25
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	1	0.25
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	1	0.25
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	1	0.25
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	1	0.25
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	1	0.25
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	1	0.25
(1,311)	1:23:A:ALA:HB1	1:51:A:THR:H	10	0.25
(1,311)	1:23:A:ALA:HB2	1:51:A:THR:H	10	0.25
(1,311)	1:23:A:ALA:HB3	1:51:A:THR:H	10	0.25
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB1	10	0.25
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB2	10	0.25
(1,269)	1:20:A:ARG:HD2	1:32:A:ALA:HB3	10	0.25
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB1	10	0.25
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB2	10	0.25
(1,269)	1:20:A:ARG:HD3	1:32:A:ALA:HB3	10	0.25
(1,263)	1:20:A:ARG:HG3	1:34:A:GLU:H	1	0.25
(1,248)	1:20:A:ARG:HB2	1:35:A:VAL:H	7	0.25
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	1	0.25
(1,185)	1:17:A:ASP:HB3	1:21:A:ALA:H	5	0.25
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	5	0.25
(2,5)	1:33:A:GLY:N	1:49:A:LEU:O	10	0.24
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	6	0.24
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	8	0.24
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	7	0.24
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	8	0.24
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD2	9	0.24
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD3	9	0.24
(1,653)	1:49:A:LEU:HB2	1:50:A:VAL:H	8	0.24
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	2	0.24
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	2	0.24
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	2	0.24
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	2	0.24
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	2	0.24
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	2	0.24
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB2	2	0.24
(1,611)	1:46:A:TYR:HE2	1:64:A:ARG:HB3	2	0.24
(1,601)	1:46:A:TYR:HB3	1:66:A:PHE:HA	4	0.24
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB2	8	0.24
(1,549)	1:44:A:ALA:HA	1:63:A:ASP:HB3	8	0.24
(1,516)	1:39:A:THR:HA	1:39:A:THR:HB	4	0.24
(1,516)	1:39:A:THR:HA	1:39:A:THR:HB	6	0.24
(1,516)	1:39:A:THR:HA	1:39:A:THR:HB	9	0.24
(1,492)	1:37:A:THR:HG21	1:46:A:TYR:HE1	2	0.24
(1,492)	1:37:A:THR:HG22	1:46:A:TYR:HE1	2	0.24
(1,492)	1:37:A:THR:HG23	1:46:A:TYR:HE1	2	0.24
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	9	0.24
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	7	0.24
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	7	0.24
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	9	0.24
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	9	0.24
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	8	0.24
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	8	0.24
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	8	0.24
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD2	8	0.24
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD3	8	0.24
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB1	5	0.24
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB2	5	0.24
(1,134)	1:15:A:ASP:HA	1:19:A:ALA:HB3	5	0.24
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	7	0.24
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	3	0.24
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	3	0.24
(2,2)	1:31:A:THR:H	1:51:A:THR:O	2	0.23
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	7	0.23
(1,984)	1:68:A:VAL:HA	1:70:A:ASP:H	3	0.23
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG11	3	0.23
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG12	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG13	3	0.23
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG21	3	0.23
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG22	3	0.23
(1,975)	1:67:A:ARG:HG2	1:68:A:VAL:HG23	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG11	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG12	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG13	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG21	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG22	3	0.23
(1,975)	1:67:A:ARG:HG3	1:68:A:VAL:HG23	3	0.23
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB2	4	0.23
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB3	4	0.23
(1,937)	1:64:A:ARG:HA	1:64:A:ARG:HG2	10	0.23
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	5	0.23
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	10	0.23
(1,809)	1:59:A:GLU:HG3	1:60:A:VAL:H	3	0.23
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	2	0.23
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	9	0.23
(1,693)	1:51:A:THR:HG21	1:54:A:ASP:H	9	0.23
(1,693)	1:51:A:THR:HG22	1:54:A:ASP:H	9	0.23
(1,693)	1:51:A:THR:HG23	1:54:A:ASP:H	9	0.23
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	2	0.23
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	2	0.23
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	9	0.23
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	9	0.23
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	9	0.23
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	9	0.23
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	9	0.23
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	9	0.23
(1,614)	1:46:A:TYR:HE2	1:66:A:PHE:HA	1	0.23
(1,612)	1:46:A:TYR:HE2	1:65:A:ASP:H	2	0.23
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	5	0.23
(1,482)	1:37:A:THR:HA	1:46:A:TYR:HD1	9	0.23
(1,450)	1:35:A:VAL:HG11	1:47:A:GLY:H	7	0.23
(1,450)	1:35:A:VAL:HG12	1:47:A:GLY:H	7	0.23
(1,450)	1:35:A:VAL:HG13	1:47:A:GLY:H	7	0.23
(1,435)	1:34:A:GLU:H	1:49:A:LEU:HD11	4	0.23
(1,435)	1:34:A:GLU:H	1:49:A:LEU:HD12	4	0.23
(1,435)	1:34:A:GLU:H	1:49:A:LEU:HD13	4	0.23
(1,371)	1:27:A:VAL:HA	1:28:A:PRO:HB3	5	0.23
(1,324)	1:24:A:VAL:HA	1:27:A:VAL:HB	2	0.23
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	6	0.23
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB1	4	0.23
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB2	4	0.23
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB3	4	0.23
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB1	4	0.23
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB2	4	0.23
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB3	4	0.23
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	9	0.23
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	9	0.23
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	9	0.23
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	6	0.23
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	6	0.23
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	6	0.23
(1,138)	1:15:A:ASP:HB3	1:18:A:ARG:H	2	0.23
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	6	0.23
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	4	0.22
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	4	0.22
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	5	0.22
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	5	0.22
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	5	0.22
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	5	0.22
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	5	0.22
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	5	0.22
(1,982)	1:68:A:VAL:HA	1:69:A:LEU:HB2	7	0.22
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	4	0.22
(1,940)	1:64:A:ARG:HB2	1:64:A:ARG:HG3	10	0.22
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	7	0.22
(1,810)	1:59:A:GLU:HG3	1:73:A:PRO:HA	5	0.22
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB1	4	0.22
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB2	4	0.22
(1,772)	1:57:A:ARG:HB2	1:74:A:ALA:HB3	4	0.22
(1,771)	1:57:A:ARG:HB2	1:74:A:ALA:H	6	0.22
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	6	0.22
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	6	0.22
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	6	0.22
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB2	7	0.22
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB2	7	0.22
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB2	7	0.22
(1,555)	1:44:A:ALA:HB1	1:61:A:HIS:HB3	7	0.22
(1,555)	1:44:A:ALA:HB2	1:61:A:HIS:HB3	7	0.22
(1,555)	1:44:A:ALA:HB3	1:61:A:HIS:HB3	7	0.22
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	10	0.22
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	10	0.22
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG11	1:49:A:LEU:HD23	1	0.22
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG12	1:49:A:LEU:HD23	1	0.22
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG13	1:49:A:LEU:HD23	1	0.22
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG21	1:49:A:LEU:HD23	1	0.22
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG22	1:49:A:LEU:HD23	1	0.22
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD21	1	0.22
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD22	1	0.22
(1,463)	1:35:A:VAL:HG23	1:49:A:LEU:HD23	1	0.22
(1,413)	1:31:A:THR:HB	1:51:A:THR:H	6	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG11	8	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG12	8	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG13	8	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG21	8	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG22	8	0.22
(1,403)	1:30:A:GLY:HA2	1:50:A:VAL:HG23	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG11	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG12	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG13	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG21	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG22	8	0.22
(1,403)	1:30:A:GLY:HA3	1:50:A:VAL:HG23	8	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG11	4	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG12	4	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG13	4	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG21	4	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG22	4	0.22
(1,360)	1:26:A:ALA:H	1:50:A:VAL:HG23	4	0.22
(1,251)	1:20:A:ARG:HB2	1:49:A:LEU:HG	10	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	9	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	9	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	9	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	9	0.22
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	9	0.22
(1,248)	1:20:A:ARG:HB2	1:35:A:VAL:H	2	0.22
(1,8)	1:3:A:MET:HG2	1:4:A:ALA:H	8	0.22
(1,1018)	1:72:A:GLU:HB2	1:73:A:PRO:HA	6	0.21
(1,1018)	1:72:A:GLU:HB3	1:73:A:PRO:HA	6	0.21
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	1	0.21
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	1	0.21
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	1	0.21
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	9	0.21
(1,776)	1:57:A:ARG:HD2	1:58:A:VAL:H	8	0.21
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD2	2	0.21
(1,761)	1:57:A:ARG:H	1:57:A:ARG:HD3	2	0.21
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	6	0.21
(1,663)	1:50:A:VAL:H	1:50:A:VAL:HB	1	0.21
(1,584)	1:46:A:TYR:HA	1:62:A:LEU:HB3	6	0.21
(1,570)	1:45:A:ALA:HB1	1:64:A:ARG:HB2	1	0.21
(1,570)	1:45:A:ALA:HB2	1:64:A:ARG:HB2	1	0.21
(1,570)	1:45:A:ALA:HB3	1:64:A:ARG:HB2	1	0.21
(1,397)	1:28:A:PRO:HD2	1:52:A:ARG:HB2	2	0.21
(1,397)	1:28:A:PRO:HD2	1:52:A:ARG:HB3	2	0.21
(1,344)	1:24:A:VAL:HG11	1:33:A:GLY:H	4	0.21
(1,344)	1:24:A:VAL:HG12	1:33:A:GLY:H	4	0.21
(1,344)	1:24:A:VAL:HG13	1:33:A:GLY:H	4	0.21
(1,344)	1:24:A:VAL:HG21	1:33:A:GLY:H	4	0.21
(1,344)	1:24:A:VAL:HG22	1:33:A:GLY:H	4	0.21
(1,344)	1:24:A:VAL:HG23	1:33:A:GLY:H	4	0.21
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	1	0.21
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	1	0.21
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	1	0.21
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	1	0.21
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	1	0.21
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	1	0.21
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	1	0.21
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	1	0.21
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	1	0.21
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	4	0.21
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	4	0.21
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	4	0.21
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	7	0.21
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	7	0.21
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	9	0.21
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	9	0.21
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	9	0.21
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	8	0.21
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	6	0.21
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	6	0.21
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	6	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG11	2	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG12	2	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG13	2	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG21	2	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG22	2	0.21
(1,157)	1:16:A:ALA:H	1:35:A:VAL:HG23	2	0.21
(1,130)	1:15:A:ASP:HA	1:18:A:ARG:HA	7	0.21
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	3	0.21
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	8	0.2
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	8	0.2
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	3	0.2
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	3	0.2
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	3	0.2
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	3	0.2
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	3	0.2
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	3	0.2
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB2	6	0.2
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB2	6	0.2
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB2	6	0.2
(1,900)	1:62:A:LEU:HD11	1:66:A:PHE:HB3	6	0.2
(1,900)	1:62:A:LEU:HD12	1:66:A:PHE:HB3	6	0.2
(1,900)	1:62:A:LEU:HD13	1:66:A:PHE:HB3	6	0.2
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	3	0.2
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	10	0.2
(1,719)	1:52:A:ARG:HB3	1:56:A:THR:HB	3	0.2
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	8	0.2
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	8	0.2
(1,640)	1:48:A:VAL:HG11	1:60:A:VAL:HA	9	0.2
(1,640)	1:48:A:VAL:HG12	1:60:A:VAL:HA	9	0.2
(1,640)	1:48:A:VAL:HG13	1:60:A:VAL:HA	9	0.2
(1,640)	1:48:A:VAL:HG21	1:60:A:VAL:HA	9	0.2
(1,640)	1:48:A:VAL:HG22	1:60:A:VAL:HA	9	0.2
(1,640)	1:48:A:VAL:HG23	1:60:A:VAL:HA	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:46:A:TYR:HD2	1:64:A:ARG:HA	1	0.2
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	6	0.2
(1,490)	1:37:A:THR:HG21	1:46:A:TYR:HA	1	0.2
(1,490)	1:37:A:THR:HG22	1:46:A:TYR:HA	1	0.2
(1,490)	1:37:A:THR:HG23	1:46:A:TYR:HA	1	0.2
(1,385)	1:27:A:VAL:HG11	1:31:A:THR:HB	8	0.2
(1,385)	1:27:A:VAL:HG12	1:31:A:THR:HB	8	0.2
(1,385)	1:27:A:VAL:HG13	1:31:A:THR:HB	8	0.2
(1,385)	1:27:A:VAL:HG21	1:31:A:THR:HB	8	0.2
(1,385)	1:27:A:VAL:HG22	1:31:A:THR:HB	8	0.2
(1,385)	1:27:A:VAL:HG23	1:31:A:THR:HB	8	0.2
(1,352)	1:25:A:GLN:HA	1:29:A:GLY:H	6	0.2
(1,264)	1:20:A:ARG:HG3	1:35:A:VAL:H	4	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG11	6	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG12	6	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG13	6	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG21	6	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG22	6	0.2
(1,259)	1:20:A:ARG:HG2	1:48:A:VAL:HG23	6	0.2
(1,53)	1:5:A:PHE:HE1	1:65:A:ASP:HA	2	0.2
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB1	8	0.2
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB2	8	0.2
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB3	8	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB1	8	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB2	8	0.2
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB3	8	0.2
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	8	0.19
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	8	0.19
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	8	0.19
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	8	0.19
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	8	0.19
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	8	0.19
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	4	0.19
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	4	0.19
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB2	4	0.19
(1,861)	1:61:A:HIS:HE1	1:70:A:ASP:HB3	4	0.19
(1,543)	1:44:A:ALA:HA	1:46:A:TYR:H	4	0.19
(1,498)	1:38:A:GLU:H	1:46:A:TYR:HB3	8	0.19
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG11	7	0.19
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG12	7	0.19
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG13	7	0.19
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG21	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG22	7	0.19
(1,378)	1:27:A:VAL:HB	1:50:A:VAL:HG23	7	0.19
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	3	0.19
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	3	0.19
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	3	0.19
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	3	0.19
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	3	0.19
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	3	0.19
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	8	0.19
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	8	0.19
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	8	0.19
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	8	0.19
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	8	0.19
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	8	0.19
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	8	0.19
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	8	0.19
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	8	0.19
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	8	0.19
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	8	0.19
(1,273)	1:21:A:ALA:H	1:24:A:VAL:H	8	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG11	2	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG12	2	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG13	2	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG21	2	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG22	2	0.19
(1,265)	1:20:A:ARG:HG3	1:48:A:VAL:HG23	2	0.19
(1,142)	1:15:A:ASP:HB2	1:18:A:ARG:HB2	6	0.19
(1,142)	1:15:A:ASP:HB3	1:18:A:ARG:HB2	6	0.19
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	1	0.19
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	5	0.19
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	5	0.19
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	5	0.19
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	5	0.19
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	5	0.19
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	5	0.19
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	6	0.19
(1,23)	1:4:A:ALA:H	1:5:A:PHE:HZ	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:79:A:GLY:H	1:80:A:LEU:H	6	0.18
(1,986)	1:68:A:VAL:HB	1:70:A:ASP:H	10	0.18
(1,920)	1:63:A:ASP:HB2	1:65:A:ASP:H	9	0.18
(1,899)	1:62:A:LEU:HD11	1:66:A:PHE:HA	10	0.18
(1,899)	1:62:A:LEU:HD12	1:66:A:PHE:HA	10	0.18
(1,899)	1:62:A:LEU:HD13	1:66:A:PHE:HA	10	0.18
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	4	0.18
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	4	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG11	10	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG12	10	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG13	10	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG21	10	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG22	10	0.18
(1,364)	1:26:A:ALA:HB1	1:50:A:VAL:HG23	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG11	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG12	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG13	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG21	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG22	10	0.18
(1,364)	1:26:A:ALA:HB2	1:50:A:VAL:HG23	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG11	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG12	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG13	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG21	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG22	10	0.18
(1,364)	1:26:A:ALA:HB3	1:50:A:VAL:HG23	10	0.18
(1,317)	1:24:A:VAL:H	1:27:A:VAL:H	7	0.18
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB1	3	0.18
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB2	3	0.18
(1,244)	1:20:A:ARG:HA	1:32:A:ALA:HB3	3	0.18
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD2	6	0.18
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD3	6	0.18
(1,122)	1:15:A:ASP:H	1:17:A:ASP:H	8	0.18
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB2	6	0.18
(1,50)	1:5:A:PHE:HD2	1:18:A:ARG:HB3	6	0.18
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB2	5	0.18
(1,43)	1:5:A:PHE:HB2	1:6:A:ASP:HB3	5	0.18
(2,3)	1:31:A:THR:O	1:51:A:THR:N	8	0.17
(1,1032)	1:79:A:GLY:H	1:80:A:LEU:H	5	0.17
(1,1023)	1:73:A:PRO:HG2	1:74:A:ALA:H	9	0.17
(1,1023)	1:73:A:PRO:HG3	1:74:A:ALA:H	9	0.17
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	7	0.17
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	7	0.17
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	7	0.17
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	7	0.17
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	7	0.17
(1,946)	1:64:A:ARG:HG2	1:66:A:PHE:H	5	0.17
(1,946)	1:64:A:ARG:HG3	1:66:A:PHE:H	5	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	5	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	5	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	5	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD21	8	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD22	8	0.17
(1,923)	1:63:A:ASP:HB2	1:69:A:LEU:HD23	8	0.17
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB2	3	0.17
(1,889)	1:62:A:LEU:HB3	1:66:A:PHE:HB3	3	0.17
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	9	0.17
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	9	0.17
(1,814)	1:59:A:GLU:HG2	1:74:A:ALA:HA	10	0.17
(1,814)	1:59:A:GLU:HG3	1:74:A:ALA:HA	10	0.17
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	3	0.17
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	3	0.17
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD2	1	0.17
(1,699)	1:51:A:THR:HG21	1:57:A:ARG:HD3	1	0.17
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD2	1	0.17
(1,699)	1:51:A:THR:HG22	1:57:A:ARG:HD3	1	0.17
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD2	1	0.17
(1,699)	1:51:A:THR:HG23	1:57:A:ARG:HD3	1	0.17
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	3	0.17
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	3	0.17
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	3	0.17
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	5	0.17
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	5	0.17
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	5	0.17
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	1	0.17
(1,676)	1:50:A:VAL:HG11	1:57:A:ARG:HG3	4	0.17
(1,676)	1:50:A:VAL:HG12	1:57:A:ARG:HG3	4	0.17
(1,676)	1:50:A:VAL:HG13	1:57:A:ARG:HG3	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:50:A:VAL:HG21	1:57:A:ARG:HG3	4	0.17
(1,676)	1:50:A:VAL:HG22	1:57:A:ARG:HG3	4	0.17
(1,676)	1:50:A:VAL:HG23	1:57:A:ARG:HG3	4	0.17
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	7	0.17
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	7	0.17
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	7	0.17
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	7	0.17
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	7	0.17
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	7	0.17
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	2	0.17
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB2	8	0.17
(1,606)	1:46:A:TYR:HD2	1:62:A:LEU:HB3	8	0.17
(1,450)	1:35:A:VAL:HG11	1:47:A:GLY:H	5	0.17
(1,450)	1:35:A:VAL:HG12	1:47:A:GLY:H	5	0.17
(1,450)	1:35:A:VAL:HG13	1:47:A:GLY:H	5	0.17
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG2	5	0.17
(1,375)	1:27:A:VAL:HA	1:52:A:ARG:HG3	5	0.17
(1,339)	1:24:A:VAL:HG11	1:30:A:GLY:H	4	0.17
(1,339)	1:24:A:VAL:HG12	1:30:A:GLY:H	4	0.17
(1,339)	1:24:A:VAL:HG13	1:30:A:GLY:H	4	0.17
(1,339)	1:24:A:VAL:HG21	1:30:A:GLY:H	4	0.17
(1,339)	1:24:A:VAL:HG22	1:30:A:GLY:H	4	0.17
(1,339)	1:24:A:VAL:HG23	1:30:A:GLY:H	4	0.17
(1,307)	1:23:A:ALA:HB1	1:48:A:VAL:H	2	0.17
(1,307)	1:23:A:ALA:HB2	1:48:A:VAL:H	2	0.17
(1,307)	1:23:A:ALA:HB3	1:48:A:VAL:H	2	0.17
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	8	0.17
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	8	0.17
(1,263)	1:20:A:ARG:HG3	1:34:A:GLU:H	4	0.17
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	1	0.17
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	1	0.17
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	1	0.17
(1,221)	1:19:A:ALA:HB1	1:20:A:ARG:H	1	0.17
(1,221)	1:19:A:ALA:HB2	1:20:A:ARG:H	1	0.17
(1,221)	1:19:A:ALA:HB3	1:20:A:ARG:H	1	0.17
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	9	0.17
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	9	0.17
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	9	0.17
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	8	0.17
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	8	0.17
(1,114)	1:14:A:PRO:HA	1:16:A:ALA:HB1	7	0.17
(1,114)	1:14:A:PRO:HA	1:16:A:ALA:HB2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:14:A:PRO:HA	1:16:A:ALA:HB3	7	0.17
(1,80)	1:9:A:ASP:HB2	1:11:A:VAL:H	5	0.17
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	4	0.16
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	1	0.16
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	2	0.16
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	2	0.16
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	2	0.16
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	2	0.16
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	2	0.16
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	2	0.16
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	8	0.16
(1,771)	1:57:A:ARG:HB2	1:74:A:ALA:H	9	0.16
(1,745)	1:54:A:ASP:HB2	1:56:A:THR:HB	5	0.16
(1,745)	1:54:A:ASP:HB3	1:56:A:THR:HB	5	0.16
(1,698)	1:51:A:THR:HG21	1:57:A:ARG:HB2	9	0.16
(1,698)	1:51:A:THR:HG22	1:57:A:ARG:HB2	9	0.16
(1,698)	1:51:A:THR:HG23	1:57:A:ARG:HB2	9	0.16
(1,668)	1:50:A:VAL:H	1:57:A:ARG:HG3	7	0.16
(1,662)	1:49:A:LEU:HD11	1:60:A:VAL:H	3	0.16
(1,662)	1:49:A:LEU:HD12	1:60:A:VAL:H	3	0.16
(1,662)	1:49:A:LEU:HD13	1:60:A:VAL:H	3	0.16
(1,662)	1:49:A:LEU:HD21	1:60:A:VAL:H	3	0.16
(1,662)	1:49:A:LEU:HD22	1:60:A:VAL:H	3	0.16
(1,662)	1:49:A:LEU:HD23	1:60:A:VAL:H	3	0.16
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD2	10	0.16
(1,654)	1:49:A:LEU:HB2	1:57:A:ARG:HD3	10	0.16
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	7	0.16
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	8	0.16
(1,485)	1:37:A:THR:HB	1:38:A:GLU:H	2	0.16
(1,398)	1:28:A:PRO:HG2	1:52:A:ARG:HA	9	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG11	6	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG12	6	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG13	6	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG21	6	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG22	6	0.16
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG23	6	0.16
(1,308)	1:23:A:ALA:HB1	1:48:A:VAL:HB	2	0.16
(1,308)	1:23:A:ALA:HB2	1:48:A:VAL:HB	2	0.16
(1,308)	1:23:A:ALA:HB3	1:48:A:VAL:HB	2	0.16
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG11	5	0.16
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG12	5	0.16
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG13	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG21	5	0.16
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG22	5	0.16
(1,301)	1:23:A:ALA:HA	1:48:A:VAL:HG23	5	0.16
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB1	10	0.16
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB2	10	0.16
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB3	10	0.16
(1,226)	1:19:A:ALA:HB1	1:47:A:GLY:H	10	0.16
(1,226)	1:19:A:ALA:HB2	1:47:A:GLY:H	10	0.16
(1,226)	1:19:A:ALA:HB3	1:47:A:GLY:H	10	0.16
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD2	5	0.16
(1,181)	1:17:A:ASP:HA	1:20:A:ARG:HD3	5	0.16
(1,180)	1:17:A:ASP:HA	1:20:A:ARG:HB3	5	0.16
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	6	0.16
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	6	0.16
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB1	6	0.16
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB2	6	0.16
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB3	6	0.16
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	9	0.16
(1,124)	1:15:A:ASP:H	1:36:A:GLU:HA	1	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	1	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	1	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	1	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	1	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	1	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	1	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	10	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	10	0.16
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	10	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	10	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	10	0.16
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	10	0.16
(1,88)	1:10:A:GLU:HA	1:11:A:VAL:HG21	6	0.16
(1,88)	1:10:A:GLU:HA	1:11:A:VAL:HG22	6	0.16
(1,88)	1:10:A:GLU:HA	1:11:A:VAL:HG23	6	0.16
(1,950)	1:65:A:ASP:HA	1:66:A:PHE:HB3	10	0.15
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	6	0.15
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	6	0.15
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	6	0.15
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	8	0.15
(1,749)	1:56:A:THR:H	1:56:A:THR:HB	2	0.15
(1,747)	1:55:A:GLY:H	1:56:A:THR:HG21	4	0.15
(1,747)	1:55:A:GLY:H	1:56:A:THR:HG22	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:55:A:GLY:H	1:56:A:THR:HG23	4	0.15
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	6	0.15
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	6	0.15
(1,543)	1:44:A:ALA:HA	1:46:A:TYR:H	8	0.15
(1,376)	1:27:A:VAL:HB	1:30:A:GLY:H	8	0.15
(1,300)	1:23:A:ALA:HA	1:27:A:VAL:H	4	0.15
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG2	6	0.15
(1,285)	1:22:A:ALA:HA	1:25:A:GLN:HG3	6	0.15
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	2	0.15
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	2	0.15
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	2	0.15
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	3	0.15
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	9	0.15
(1,160)	1:16:A:ALA:HA	1:19:A:ALA:H	6	0.15
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB2	2	0.15
(1,156)	1:16:A:ALA:H	1:34:A:GLU:HB3	2	0.15
(1,135)	1:15:A:ASP:HB2	1:18:A:ARG:H	4	0.15
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	2	0.15
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	9	0.15
(1,950)	1:65:A:ASP:HA	1:66:A:PHE:HB3	1	0.14
(1,950)	1:65:A:ASP:HA	1:66:A:PHE:HB3	9	0.14
(1,937)	1:64:A:ARG:HA	1:64:A:ARG:HG2	3	0.14
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	7	0.14
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	5	0.14
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	2	0.14
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	2	0.14
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	2	0.14
(1,693)	1:51:A:THR:HG21	1:54:A:ASP:H	2	0.14
(1,693)	1:51:A:THR:HG22	1:54:A:ASP:H	2	0.14
(1,693)	1:51:A:THR:HG23	1:54:A:ASP:H	2	0.14
(1,653)	1:49:A:LEU:HB2	1:50:A:VAL:H	6	0.14
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	2	0.14
(1,278)	1:21:A:ALA:HA	1:25:A:GLN:HE21	1	0.14
(1,278)	1:21:A:ALA:HA	1:25:A:GLN:HE22	1	0.14
(1,276)	1:21:A:ALA:HA	1:24:A:VAL:HB	5	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	8	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	8	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	8	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	8	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	8	0.14
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	8	0.14
(1,243)	1:20:A:ARG:HA	1:24:A:VAL:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:18:A:ARG:HB3	1:66:A:PHE:HD1	9	0.14
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB1	2	0.14
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB2	2	0.14
(1,155)	1:16:A:ALA:H	1:19:A:ALA:HB3	2	0.14
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	8	0.14
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	6	0.14
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	6	0.14
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	6	0.14
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	6	0.14
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	6	0.14
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	6	0.14
(1,36)	1:5:A:PHE:HA	1:66:A:PHE:HD1	9	0.14
(1,1019)	1:72:A:GLU:HB2	1:73:A:PRO:HD2	1	0.13
(1,1019)	1:72:A:GLU:HB3	1:73:A:PRO:HD2	1	0.13
(1,988)	1:68:A:VAL:HG11	1:70:A:ASP:H	5	0.13
(1,988)	1:68:A:VAL:HG12	1:70:A:ASP:H	5	0.13
(1,988)	1:68:A:VAL:HG13	1:70:A:ASP:H	5	0.13
(1,988)	1:68:A:VAL:HG21	1:70:A:ASP:H	5	0.13
(1,988)	1:68:A:VAL:HG22	1:70:A:ASP:H	5	0.13
(1,988)	1:68:A:VAL:HG23	1:70:A:ASP:H	5	0.13
(1,946)	1:64:A:ARG:HG2	1:66:A:PHE:H	4	0.13
(1,946)	1:64:A:ARG:HG3	1:66:A:PHE:H	4	0.13
(1,946)	1:64:A:ARG:HG2	1:66:A:PHE:H	7	0.13
(1,946)	1:64:A:ARG:HG3	1:66:A:PHE:H	7	0.13
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD21	2	0.13
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD22	2	0.13
(1,929)	1:63:A:ASP:HB3	1:69:A:LEU:HD23	2	0.13
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	3	0.13
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	4	0.13
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	10	0.13
(1,773)	1:57:A:ARG:HB3	1:57:A:ARG:HG2	9	0.13
(1,758)	1:56:A:THR:HG21	1:57:A:ARG:H	5	0.13
(1,758)	1:56:A:THR:HG22	1:57:A:ARG:H	5	0.13
(1,758)	1:56:A:THR:HG23	1:57:A:ARG:H	5	0.13
(1,730)	1:52:A:ARG:HD2	1:56:A:THR:HB	8	0.13
(1,730)	1:52:A:ARG:HD3	1:56:A:THR:HB	8	0.13
(1,681)	1:51:A:THR:H	1:51:A:THR:HG21	1	0.13
(1,681)	1:51:A:THR:H	1:51:A:THR:HG22	1	0.13
(1,681)	1:51:A:THR:H	1:51:A:THR:HG23	1	0.13
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	1	0.13
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	1	0.13
(1,653)	1:49:A:LEU:HB2	1:50:A:VAL:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:46:A:TYR:HE2	1:66:A:PHE:HB2	6	0.13
(1,584)	1:46:A:TYR:HA	1:62:A:LEU:HB3	2	0.13
(1,579)	1:46:A:TYR:H	1:63:A:ASP:H	2	0.13
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB2	7	0.13
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB2	7	0.13
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB2	7	0.13
(1,558)	1:44:A:ALA:HB1	1:69:A:LEU:HB3	7	0.13
(1,558)	1:44:A:ALA:HB2	1:69:A:LEU:HB3	7	0.13
(1,558)	1:44:A:ALA:HB3	1:69:A:LEU:HB3	7	0.13
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB1	7	0.13
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB2	7	0.13
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB3	7	0.13
(1,506)	1:38:A:GLU:HB2	1:40:A:GLY:H	1	0.13
(1,506)	1:38:A:GLU:HB3	1:40:A:GLY:H	1	0.13
(1,489)	1:37:A:THR:HG21	1:46:A:TYR:H	8	0.13
(1,489)	1:37:A:THR:HG22	1:46:A:TYR:H	8	0.13
(1,489)	1:37:A:THR:HG23	1:46:A:TYR:H	8	0.13
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	6	0.13
(1,458)	1:35:A:VAL:HG11	1:47:A:GLY:H	5	0.13
(1,458)	1:35:A:VAL:HG12	1:47:A:GLY:H	5	0.13
(1,458)	1:35:A:VAL:HG13	1:47:A:GLY:H	5	0.13
(1,458)	1:35:A:VAL:HG21	1:47:A:GLY:H	5	0.13
(1,458)	1:35:A:VAL:HG22	1:47:A:GLY:H	5	0.13
(1,458)	1:35:A:VAL:HG23	1:47:A:GLY:H	5	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG11	4	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG12	4	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG13	4	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG21	4	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG22	4	0.13
(1,423)	1:32:A:ALA:HB1	1:50:A:VAL:HG23	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG11	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG12	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG13	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG21	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG22	4	0.13
(1,423)	1:32:A:ALA:HB2	1:50:A:VAL:HG23	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG11	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG12	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG13	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG21	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG22	4	0.13
(1,423)	1:32:A:ALA:HB3	1:50:A:VAL:HG23	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:30:A:GLY:H	1:31:A:THR:H	10	0.13
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	1	0.13
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	7	0.13
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB1	1	0.13
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB2	1	0.13
(1,260)	1:20:A:ARG:HG3	1:32:A:ALA:HB3	1	0.13
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB1	5	0.13
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB2	5	0.13
(1,255)	1:20:A:ARG:HB3	1:32:A:ALA:HB3	5	0.13
(1,224)	1:19:A:ALA:HB1	1:35:A:VAL:H	7	0.13
(1,224)	1:19:A:ALA:HB2	1:35:A:VAL:H	7	0.13
(1,224)	1:19:A:ALA:HB3	1:35:A:VAL:H	7	0.13
(1,209)	1:18:A:ARG:HG2	1:20:A:ARG:H	6	0.13
(1,167)	1:16:A:ALA:HB1	1:17:A:ASP:HB2	8	0.13
(1,167)	1:16:A:ALA:HB2	1:17:A:ASP:HB2	8	0.13
(1,167)	1:16:A:ALA:HB3	1:17:A:ASP:HB2	8	0.13
(1,103)	1:12:A:THR:HA	1:13:A:GLY:H	7	0.13
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	3	0.13
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	3	0.13
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	3	0.13
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	1	0.13
(1,11)	1:3:A:MET:HG3	1:4:A:ALA:H	10	0.13
(2,4)	1:31:A:THR:O	1:51:A:THR:H	7	0.12
(1,1032)	1:79:A:GLY:H	1:80:A:LEU:H	1	0.12
(1,987)	1:68:A:VAL:HG11	1:69:A:LEU:H	6	0.12
(1,987)	1:68:A:VAL:HG12	1:69:A:LEU:H	6	0.12
(1,987)	1:68:A:VAL:HG13	1:69:A:LEU:H	6	0.12
(1,987)	1:68:A:VAL:HG21	1:69:A:LEU:H	6	0.12
(1,987)	1:68:A:VAL:HG22	1:69:A:LEU:H	6	0.12
(1,987)	1:68:A:VAL:HG23	1:69:A:LEU:H	6	0.12
(1,984)	1:68:A:VAL:HA	1:70:A:ASP:H	4	0.12
(1,902)	1:62:A:LEU:HD11	1:67:A:ARG:HA	2	0.12
(1,902)	1:62:A:LEU:HD12	1:67:A:ARG:HA	2	0.12
(1,902)	1:62:A:LEU:HD13	1:67:A:ARG:HA	2	0.12
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	6	0.12
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB1	10	0.12
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB2	10	0.12
(1,781)	1:57:A:ARG:HD2	1:74:A:ALA:HB3	10	0.12
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB1	10	0.12
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB2	10	0.12
(1,781)	1:57:A:ARG:HD3	1:74:A:ALA:HB3	10	0.12
(1,695)	1:51:A:THR:HG21	1:55:A:GLY:HA2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:51:A:THR:HG22	1:55:A:GLY:HA2	1	0.12
(1,695)	1:51:A:THR:HG23	1:55:A:GLY:HA2	1	0.12
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB2	10	0.12
(1,667)	1:50:A:VAL:H	1:57:A:ARG:HB3	10	0.12
(1,663)	1:50:A:VAL:H	1:50:A:VAL:HB	4	0.12
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD21	1	0.12
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD22	1	0.12
(1,618)	1:47:A:GLY:H	1:62:A:LEU:HD23	1	0.12
(1,584)	1:46:A:TYR:HA	1:62:A:LEU:HB3	3	0.12
(1,486)	1:37:A:THR:HB	1:46:A:TYR:HA	5	0.12
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB1	9	0.12
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB2	9	0.12
(1,331)	1:24:A:VAL:HG11	1:32:A:ALA:HB3	9	0.12
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB1	9	0.12
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB2	9	0.12
(1,331)	1:24:A:VAL:HG12	1:32:A:ALA:HB3	9	0.12
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB1	9	0.12
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB2	9	0.12
(1,331)	1:24:A:VAL:HG13	1:32:A:ALA:HB3	9	0.12
(1,292)	1:23:A:ALA:H	1:26:A:ALA:H	9	0.12
(1,291)	1:23:A:ALA:H	1:25:A:GLN:H	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG11	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG12	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG13	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG21	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG22	6	0.12
(1,249)	1:20:A:ARG:HB2	1:48:A:VAL:HG23	6	0.12
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	3	0.12
(1,35)	1:5:A:PHE:HA	1:5:A:PHE:HE2	4	0.12
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	1	0.12
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	1	0.12
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	1	0.12
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	2	0.12
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	2	0.12
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	2	0.12
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	9	0.12
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	9	0.12
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	9	0.12
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB1	4	0.12
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB2	4	0.12
(1,16)	1:3:A:MET:HB2	1:4:A:ALA:HB3	4	0.12
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB1	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB2	4	0.12
(1,16)	1:3:A:MET:HB3	1:4:A:ALA:HB3	4	0.12
(1,13)	1:3:A:MET:HG3	1:5:A:PHE:HZ	2	0.12
(1,1018)	1:72:A:GLU:HB2	1:73:A:PRO:HA	3	0.11
(1,1018)	1:72:A:GLU:HB3	1:73:A:PRO:HA	3	0.11
(1,881)	1:62:A:LEU:HB2	1:66:A:PHE:HA	1	0.11
(1,880)	1:62:A:LEU:HB2	1:63:A:ASP:H	4	0.11
(1,872)	1:62:A:LEU:HA	1:66:A:PHE:HA	7	0.11
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	6	0.11
(1,865)	1:62:A:LEU:H	1:62:A:LEU:HG	8	0.11
(1,838)	1:61:A:HIS:H	1:68:A:VAL:HA	1	0.11
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	7	0.11
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	10	0.11
(1,823)	1:60:A:VAL:HA	1:72:A:GLU:H	3	0.11
(1,778)	1:57:A:ARG:HD3	1:58:A:VAL:H	10	0.11
(1,704)	1:52:A:ARG:H	1:56:A:THR:H	4	0.11
(1,663)	1:50:A:VAL:H	1:50:A:VAL:HB	2	0.11
(1,663)	1:50:A:VAL:H	1:50:A:VAL:HB	7	0.11
(1,655)	1:49:A:LEU:HB3	1:49:A:LEU:HG	10	0.11
(1,594)	1:46:A:TYR:HB3	1:46:A:TYR:HD1	3	0.11
(1,580)	1:46:A:TYR:H	1:63:A:ASP:HA	6	0.11
(1,580)	1:46:A:TYR:H	1:63:A:ASP:HA	10	0.11
(1,571)	1:45:A:ALA:HB1	1:64:A:ARG:HG2	10	0.11
(1,571)	1:45:A:ALA:HB2	1:64:A:ARG:HG2	10	0.11
(1,571)	1:45:A:ALA:HB3	1:64:A:ARG:HG2	10	0.11
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB2	10	0.11
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB2	10	0.11
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB2	10	0.11
(1,568)	1:45:A:ALA:HB1	1:63:A:ASP:HB3	10	0.11
(1,568)	1:45:A:ALA:HB2	1:63:A:ASP:HB3	10	0.11
(1,568)	1:45:A:ALA:HB3	1:63:A:ASP:HB3	10	0.11
(1,546)	1:44:A:ALA:HA	1:62:A:LEU:HB2	1	0.11
(1,473)	1:36:A:GLU:HG3	1:47:A:GLY:H	4	0.11
(1,365)	1:27:A:VAL:H	1:27:A:VAL:HB	3	0.11
(1,342)	1:24:A:VAL:HG11	1:32:A:ALA:H	8	0.11
(1,342)	1:24:A:VAL:HG12	1:32:A:ALA:H	8	0.11
(1,342)	1:24:A:VAL:HG13	1:32:A:ALA:H	8	0.11
(1,342)	1:24:A:VAL:HG21	1:32:A:ALA:H	8	0.11
(1,342)	1:24:A:VAL:HG22	1:32:A:ALA:H	8	0.11
(1,342)	1:24:A:VAL:HG23	1:32:A:ALA:H	8	0.11
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG11	1:27:A:VAL:HG23	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG12	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG12	1:27:A:VAL:HG23	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG12	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG13	1:27:A:VAL:HG23	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG12	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG21	1:27:A:VAL:HG23	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG12	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG22	1:27:A:VAL:HG23	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG11	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG12	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG13	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG21	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG22	10	0.11
(1,338)	1:24:A:VAL:HG23	1:27:A:VAL:HG23	10	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG11	8	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG12	8	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG13	8	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG21	8	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG22	8	0.11
(1,325)	1:24:A:VAL:HA	1:27:A:VAL:HG23	8	0.11
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG11	7	0.11
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG12	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG13	7	0.11
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG21	7	0.11
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG22	7	0.11
(1,305)	1:23:A:ALA:HB1	1:24:A:VAL:HG23	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG11	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG12	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG13	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG21	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG22	7	0.11
(1,305)	1:23:A:ALA:HB2	1:24:A:VAL:HG23	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG11	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG12	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG13	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG21	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG22	7	0.11
(1,305)	1:23:A:ALA:HB3	1:24:A:VAL:HG23	7	0.11
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD11	7	0.11
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD12	7	0.11
(1,246)	1:20:A:ARG:HA	1:49:A:LEU:HD13	7	0.11
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB1	7	0.11
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB2	7	0.11
(1,242)	1:20:A:ARG:HA	1:23:A:ALA:HB3	7	0.11
(1,215)	1:19:A:ALA:H	1:21:A:ALA:H	8	0.11
(1,209)	1:18:A:ARG:HG2	1:20:A:ARG:H	2	0.11
(1,201)	1:18:A:ARG:HB2	1:66:A:PHE:HD1	1	0.11
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB1	1	0.11
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB2	1	0.11
(1,197)	1:18:A:ARG:HA	1:21:A:ALA:HB3	1	0.11
(1,129)	1:15:A:ASP:HA	1:18:A:ARG:H	2	0.11
(1,91)	1:10:A:GLU:HG2	1:11:A:VAL:H	7	0.11
(1,91)	1:10:A:GLU:HG3	1:11:A:VAL:H	7	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	2	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	2	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	2	0.11
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	2	0.11
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	2	0.11
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	2	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG21	9	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG22	9	0.11
(1,90)	1:10:A:GLU:HB2	1:11:A:VAL:HG23	9	0.11
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG21	9	0.11
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:10:A:GLU:HB3	1:11:A:VAL:HG23	9	0.11
(1,82)	1:9:A:ASP:HB3	1:11:A:VAL:H	6	0.11
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	8	0.11
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	8	0.11
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	8	0.11
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	10	0.11
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	10	0.11
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	10	0.11
(1,973)	1:67:A:ARG:HG2	1:68:A:VAL:H	1	0.1
(1,973)	1:67:A:ARG:HG3	1:68:A:VAL:H	1	0.1
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB2	1	0.1
(1,959)	1:66:A:PHE:H	1:67:A:ARG:HB3	1	0.1
(1,827)	1:60:A:VAL:HB	1:71:A:THR:HA	4	0.1
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD2	4	0.1
(1,660)	1:49:A:LEU:HD11	1:57:A:ARG:HD3	4	0.1
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD2	4	0.1
(1,660)	1:49:A:LEU:HD12	1:57:A:ARG:HD3	4	0.1
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD2	4	0.1
(1,660)	1:49:A:LEU:HD13	1:57:A:ARG:HD3	4	0.1
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB1	8	0.1
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB2	8	0.1
(1,530)	1:42:A:GLY:H	1:43:A:ALA:HB3	8	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG11	3	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG12	3	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG13	3	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG21	3	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG22	3	0.1
(1,425)	1:33:A:GLY:H	1:48:A:VAL:HG23	3	0.1
(1,308)	1:23:A:ALA:HB1	1:48:A:VAL:HB	9	0.1
(1,308)	1:23:A:ALA:HB2	1:48:A:VAL:HB	9	0.1
(1,308)	1:23:A:ALA:HB3	1:48:A:VAL:HB	9	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	6	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	6	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	6	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB1	7	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB2	7	0.1
(1,234)	1:20:A:ARG:H	1:32:A:ALA:HB3	7	0.1
(1,163)	1:16:A:ALA:HA	1:35:A:VAL:HB	6	0.1
(1,158)	1:16:A:ALA:HA	1:17:A:ASP:HA	8	0.1
(1,107)	1:13:A:GLY:H	1:16:A:ALA:HB1	8	0.1
(1,107)	1:13:A:GLY:H	1:16:A:ALA:HB2	8	0.1
(1,107)	1:13:A:GLY:H	1:16:A:ALA:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG21	9	0.1
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG22	9	0.1
(1,83)	1:9:A:ASP:HB3	1:11:A:VAL:HG23	9	0.1
(1,77)	1:9:A:ASP:HA	1:10:A:GLU:H	9	0.1
(1,26)	1:4:A:ALA:HB1	1:5:A:PHE:H	7	0.1
(1,26)	1:4:A:ALA:HB2	1:5:A:PHE:H	7	0.1
(1,26)	1:4:A:ALA:HB3	1:5:A:PHE:H	7	0.1
(1,14)	1:3:A:MET:HB2	1:3:A:MET:HG3	8	0.1
(1,14)	1:3:A:MET:HB3	1:3:A:MET:HG3	8	0.1
(1,14)	1:3:A:MET:HB2	1:3:A:MET:HG3	10	0.1
(1,14)	1:3:A:MET:HB3	1:3:A:MET:HG3	10	0.1

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

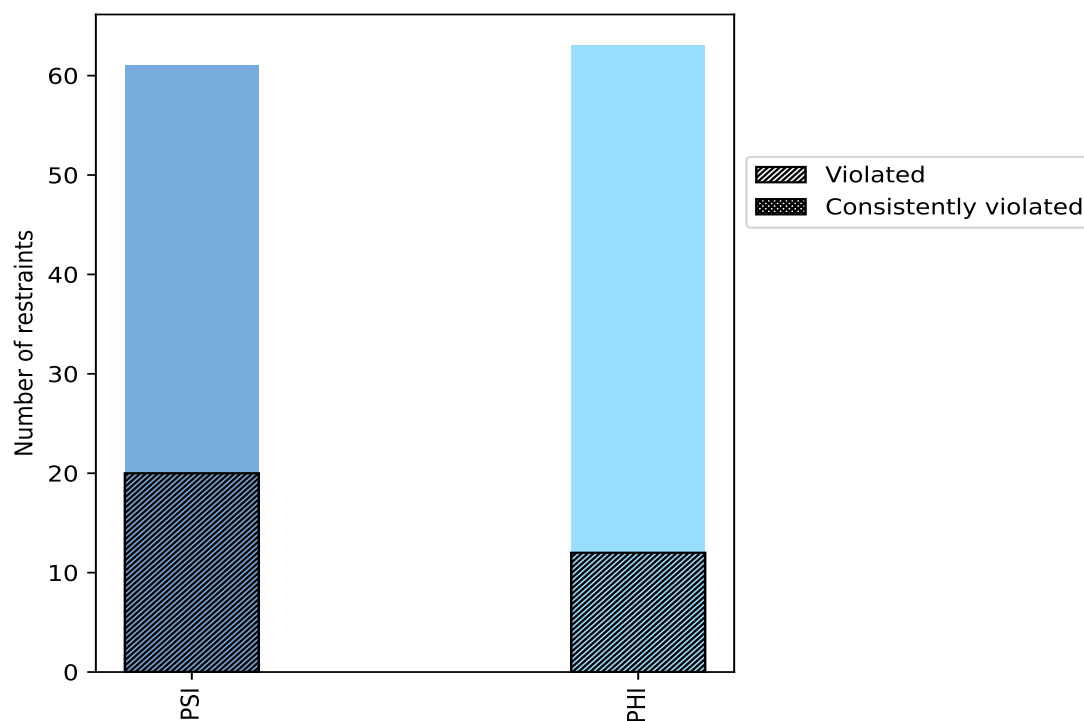
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	61	49.2	20	32.8	16.1	0	0.0	0.0
PHI	63	50.8	12	19.0	9.7	0	0.0	0.0
Total	124	100.0	32	25.8	25.8	0	0.0	0.0

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

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



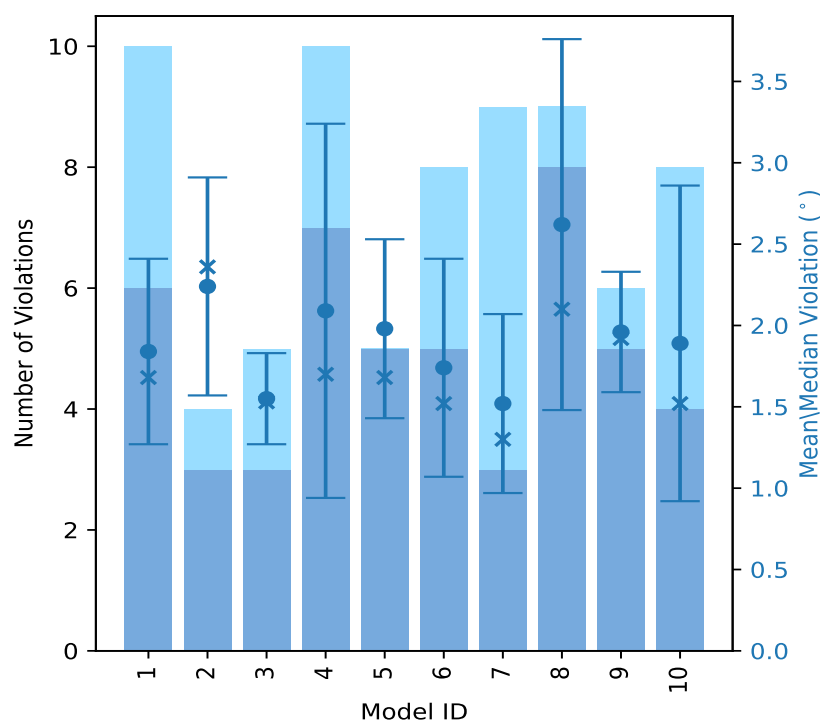
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	4	10	1.84	2.71	0.57	1.68
2	3	1	4	2.24	3.05	0.67	2.36
3	3	2	5	1.55	1.97	0.28	1.53
4	7	3	10	2.09	4.83	1.15	1.7
5	5	0	5	1.98	2.79	0.55	1.68
6	5	3	8	1.74	2.88	0.67	1.52
7	3	6	9	1.52	3.0	0.55	1.3
8	8	1	9	2.62	4.58	1.14	2.1
9	5	1	6	1.96	2.53	0.37	1.92
10	4	4	8	1.89	4.1	0.97	1.52

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



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

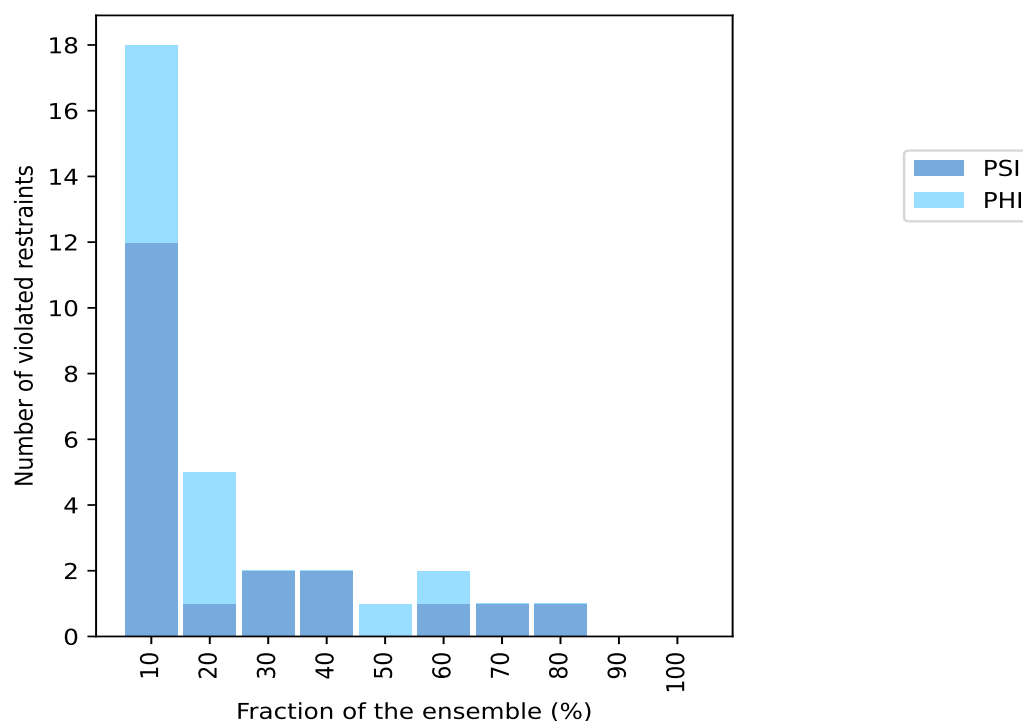
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
12	6	18	1	10.0
1	4	5	2	20.0
2	0	2	3	30.0
2	0	2	4	40.0
0	1	1	5	50.0
1	1	2	6	60.0
1	0	1	7	70.0
1	0	1	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

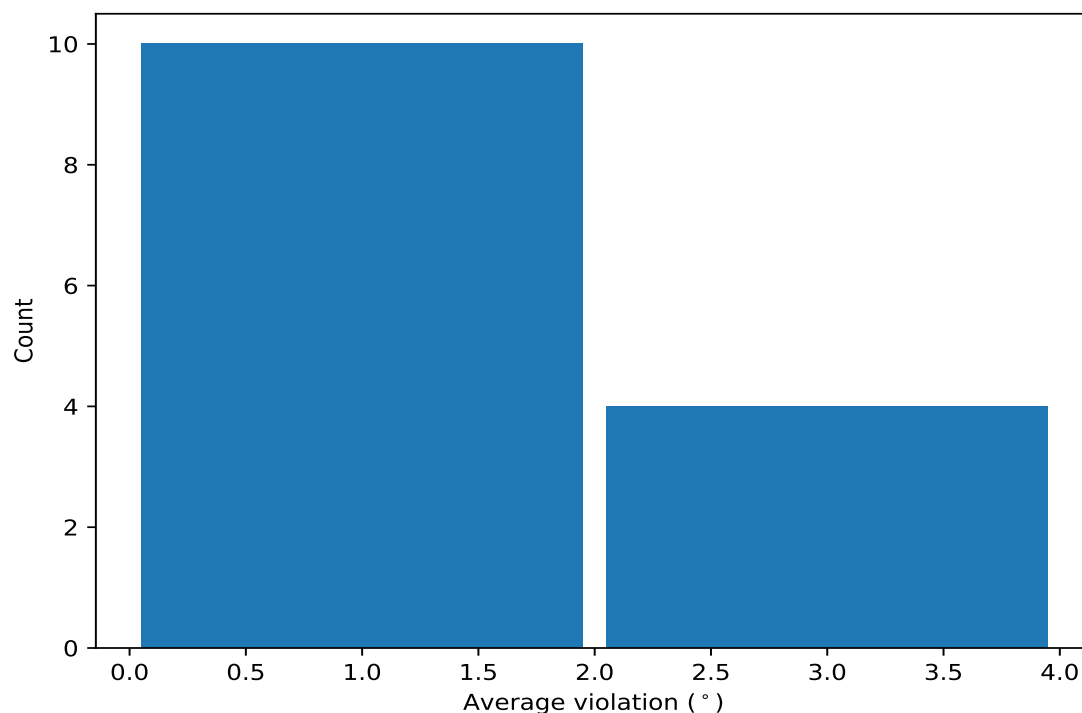
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	8	2.58	0.77	2.62
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	7	1.89	0.26	1.91
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	6	2.21	1.14	1.69
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	6	1.96	0.34	1.94
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	5	1.92	0.92	1.63
(1,51)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:GLU:N	4	1.85	0.36	1.67
(1,69)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:GLY:N	4	1.49	0.35	1.38
(1,57)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:THR:N	3	3.01	1.5	3.05
(1,85)	1:55:A:GLY:N	1:55:A:GLY:CA	1:55:A:GLY:C	1:56:A:THR:N	3	1.39	0.14	1.41
(1,61)	1:38:A:GLU:N	1:38:A:GLU:CA	1:38:A:GLU:C	1:39:A:THR:N	2	2.02	0.37	2.02
(1,56)	1:35:A:VAL:C	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	2	1.98	0.4	1.98
(1,54)	1:34:A:GLU:C	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	2	1.44	0.24	1.44
(1,16)	1:11:A:VAL:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	2	1.43	0.31	1.43

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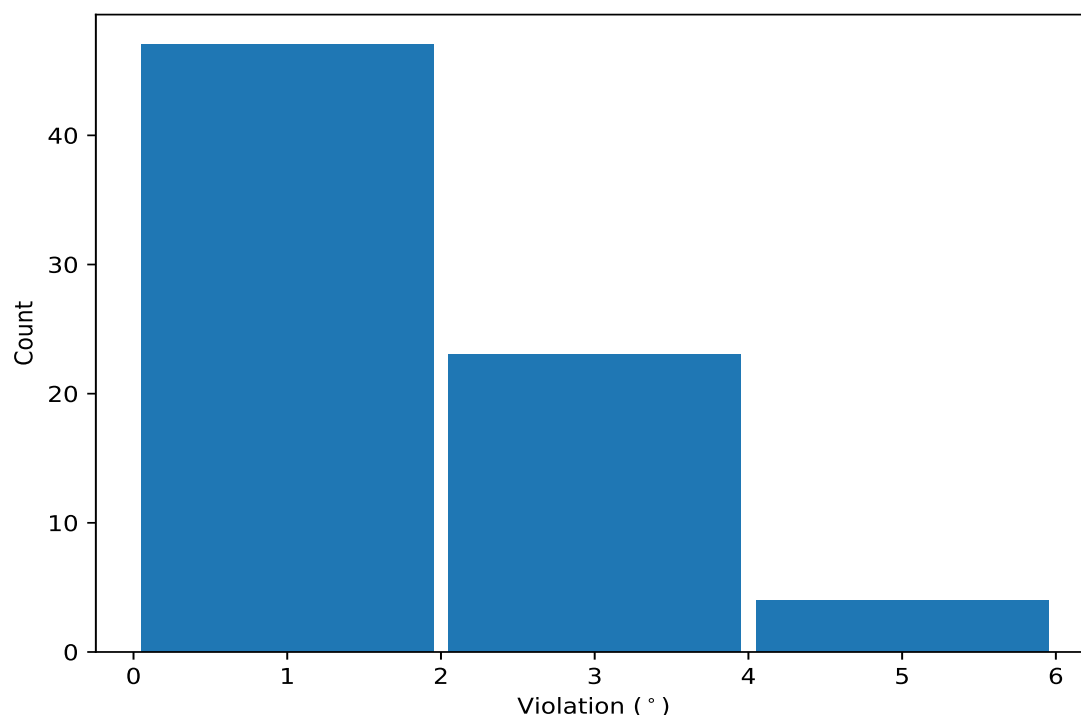
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,119)	1:76:A:GLY:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	2	1.23	0.07	1.23

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:THR:N	4	4.83
(1,19)	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	1:16:A:ALA:N	8	4.58
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	8	4.51
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	10	4.1
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	4	3.58
(1,10)	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	1:9:A:ASP:N	8	3.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:THR:N	2	3.05
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	7	3.0
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	6	2.88
(1,120)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:GLY:N	5	2.79
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	6	2.75
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	1	2.71
(1,62)	1:38:A:GLU:C	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1	2.65
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	2	2.54
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	9	2.53
(1,51)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:GLU:N	5	2.47
(1,61)	1:38:A:GLU:N	1:38:A:GLU:CA	1:38:A:GLU:C	1:39:A:THR:N	1	2.39
(1,56)	1:35:A:VAL:C	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	10	2.39
(1,17)	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	1:14:A:PRO:N	8	2.3
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	9	2.22
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	10	2.21
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	2	2.18
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	9	2.17
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	1	2.14
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	4	2.12
(1,89)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	1:58:A:VAL:N	8	2.1
(1,69)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:GLY:N	4	2.06
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	3	1.97
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	8	1.91
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	6	1.9
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	10	1.84
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	8	1.77
(1,16)	1:11:A:VAL:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	4	1.74
(1,51)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:GLU:N	1	1.73
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	3	1.7
(1,54)	1:34:A:GLU:C	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	8	1.69
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	5	1.68
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	4	1.67
(1,61)	1:38:A:GLU:N	1:38:A:GLU:CA	1:38:A:GLU:C	1:39:A:THR:N	9	1.66
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	1	1.63
(1,51)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:GLU:N	9	1.61
(1,56)	1:35:A:VAL:C	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	7	1.58
(1,51)	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1:34:A:GLU:N	7	1.58
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	9	1.57
(1,85)	1:55:A:GLY:N	1:55:A:GLY:CA	1:55:A:GLY:C	1:56:A:THR:N	5	1.56
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	6	1.56
(1,122)	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	1:80:A:LEU:N	3	1.53
(1,100)	1:62:A:LEU:C	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1	1.51
(1,69)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:GLY:N	6	1.47
(1,71)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:VAL:N	7	1.46
(1,55)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:GLU:N	4	1.42
(1,39)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:ALA:N	8	1.42
(1,85)	1:55:A:GLY:N	1:55:A:GLY:CA	1:55:A:GLY:C	1:56:A:THR:N	3	1.41
(1,12)	1:9:A:ASP:N	1:9:A:ASP:CA	1:9:A:ASP:C	1:10:A:GLU:N	4	1.39
(1,112)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:GLU:N	5	1.38
(1,65)	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	1:42:A:GLY:N	1	1.31
(1,119)	1:76:A:GLY:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	7	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:GLY:N	1	1.28
(1,18)	1:14:A:PRO:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	7	1.25
(1,117)	1:74:A:ALA:C	1:75:A:ASP:N	1:75:A:ASP:CA	1:75:A:ASP:C	7	1.23
(1,85)	1:55:A:GLY:N	1:55:A:GLY:CA	1:55:A:GLY:C	1:56:A:THR:N	2	1.21
(1,54)	1:34:A:GLU:C	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	10	1.2
(1,119)	1:76:A:GLY:C	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	6	1.16
(1,69)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:GLY:N	10	1.16
(1,57)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:THR:N	6	1.16
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	7	1.15
(1,121)	1:78:A:GLY:C	1:79:A:GLY:N	1:79:A:GLY:CA	1:79:A:GLY:C	10	1.13
(1,16)	1:11:A:VAL:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	3	1.12
(1,68)	1:45:A:ALA:C	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	7	1.09
(1,59)	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	1:38:A:GLU:N	10	1.07
(1,58)	1:36:A:GLU:C	1:37:A:THR:N	1:37:A:THR:CA	1:37:A:THR:C	6	1.06
(1,8)	1:5:A:PHE:N	1:5:A:PHE:CA	1:5:A:PHE:C	1:6:A:ASP:N	4	1.06
(1,94)	1:59:A:GLU:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1	1.03
(1,63)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	4	1.0