



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 AM UTC

PDB ID : 5XE4 / pdb_00005xe4
BMRB ID : 36070
Title : NMR solution structure of the aromatic mutant H43W H67F cytochrome b5
Authors : Balakrishnan, S.; Sarma, S.P.
Deposited on : 2017-03-31

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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

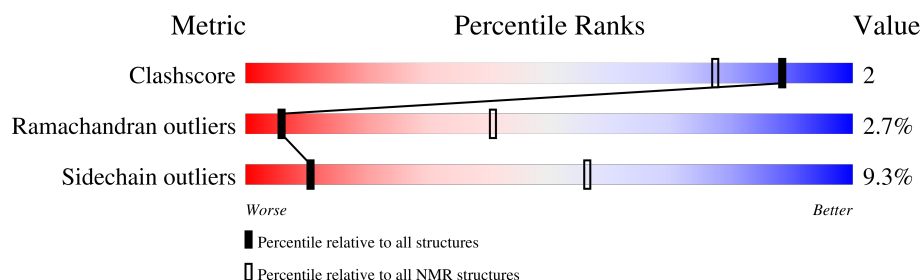
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 68%.

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	98	 88% 9% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:98 (96)	0.59	6

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1571 atoms, of which 772 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome b5.

Mol	Chain	Residues	Atoms					Trace
1	A	98	Total	C	H	N	O	0
			1571	503	772	132	164	

There are 3 discrepancies between the modelled and reference sequences:

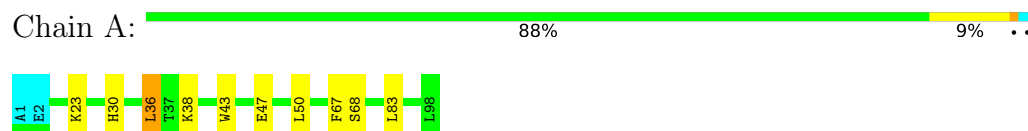
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	TRP	HIS	engineered mutation	UNP P00173
A	67	PHE	HIS	engineered mutation	UNP P00173
A	77	LYS	THR	engineered mutation	UNP P00173

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: Cytochrome b5

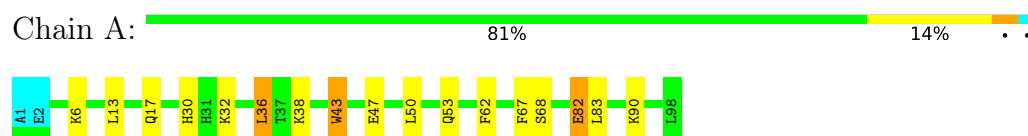


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

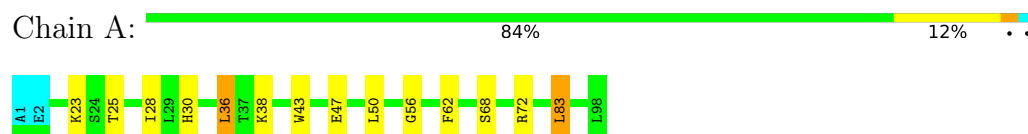
4.2.1 Score per residue for model 1

- Molecule 1: Cytochrome b5



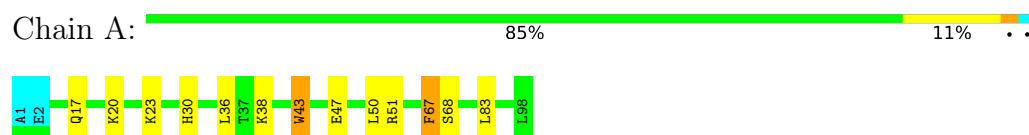
4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome b5



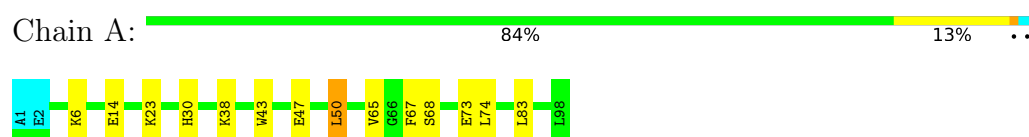
4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome b5



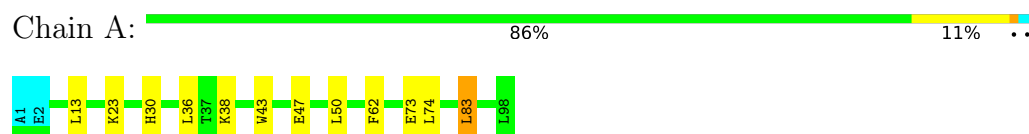
4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome b5



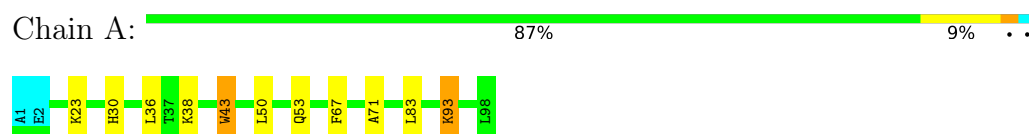
4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome b5



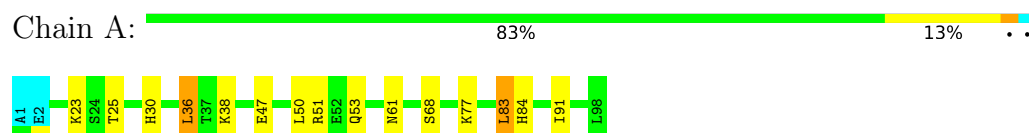
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Cytochrome b5



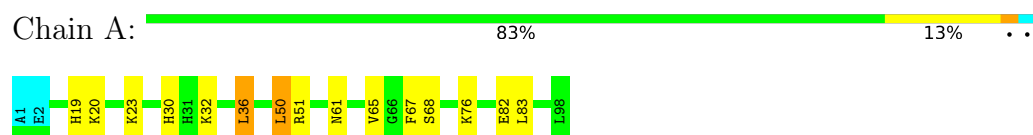
4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome b5



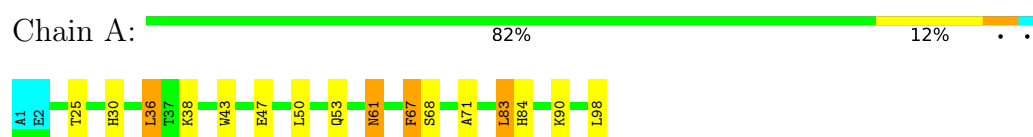
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome b5



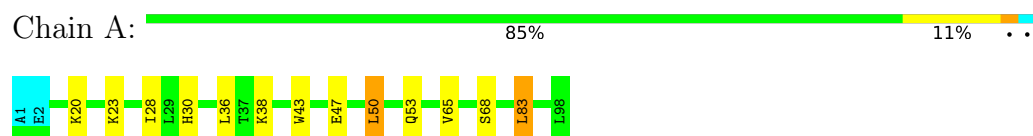
4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome b5



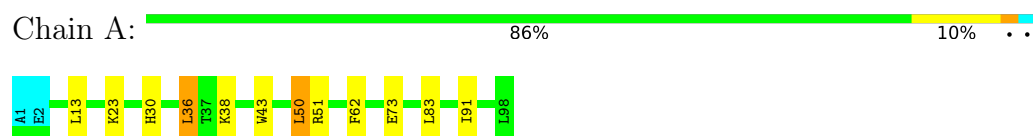
4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome b5



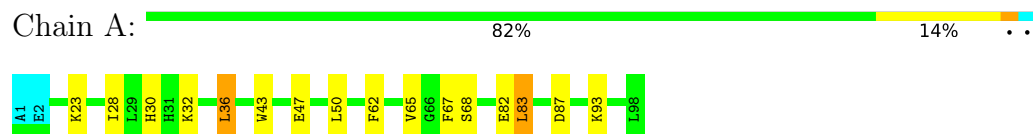
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome b5



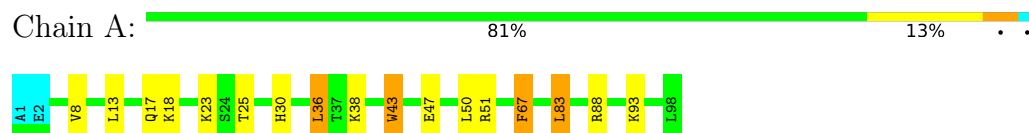
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome b5



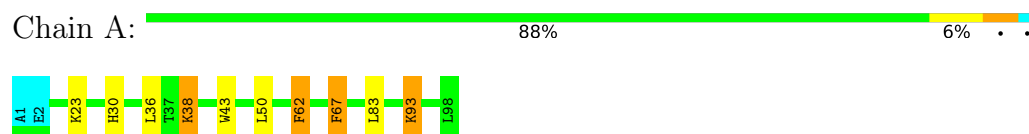
4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome b5



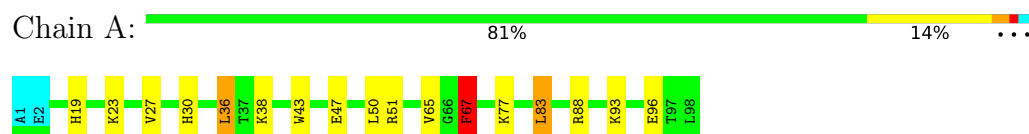
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome b5



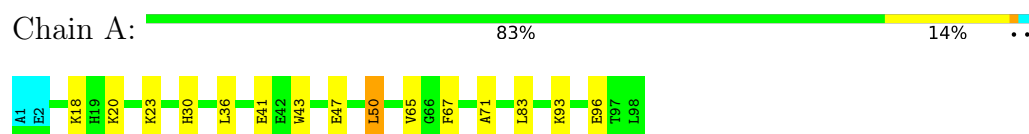
4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome b5



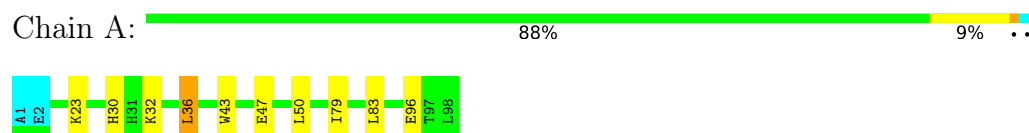
4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome b5



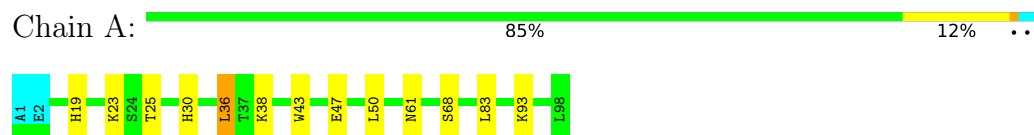
4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome b5



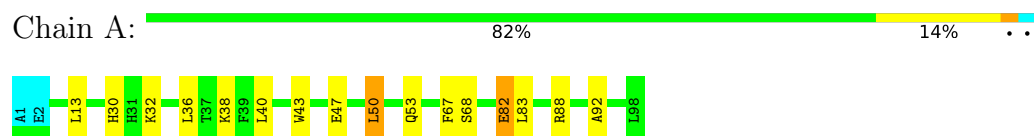
4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome b5



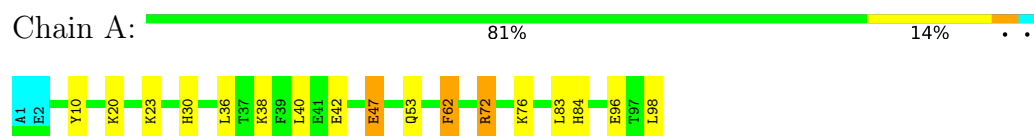
4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome b5



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome b5



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	920
Number of shifts mapped to atoms	920
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.19±0.02	0±0/802 (0.0± 0.0%)	1.00±0.03	0±1/1079 (0.0± 0.1%)
All	All	1.19	4/16040 (0.0%)	1.00	6/21580 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	43	TRP	C-N	5.81	1.41	1.34	1	4

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	ASN	CA-CB-CG	5.77	118.37	112.60	9	2
1	A	67	PHE	CA-CB-CG	5.76	119.56	113.80	15	2
1	A	62	PHE	CA-CB-CG	5.33	119.14	113.80	14	2

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	785	759	755	3±1
All	All	15700	15180	15100	60

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HB3	1:A:65:VAL:HB	0.57	1.76	12	5
1:A:73:GLU:HG3	1:A:74:LEU:HD22	0.51	1.82	4	2
1:A:19:HIS:HB2	1:A:51:ARG:HG2	0.51	1.82	8	2
1:A:36:LEU:HD12	1:A:50:LEU:HD13	0.48	1.85	15	8
1:A:40:LEU:HD13	1:A:47:GLU:HB3	0.48	1.85	20	1
1:A:25:THR:HG22	1:A:36:LEU:HB3	0.47	1.86	18	5
1:A:67:PHE:HB2	1:A:71:ALA:HB2	0.47	1.86	9	3
1:A:32:LYS:HA	1:A:82:GLU:HA	0.47	1.86	8	4
1:A:20:LYS:HA	1:A:51:ARG:HD2	0.46	1.85	3	1
1:A:32:LYS:NZ	1:A:79:ILE:HD11	0.45	2.26	17	1
1:A:28:ILE:HG21	1:A:83:LEU:HG	0.45	1.88	10	3
1:A:27:VAL:HG22	1:A:36:LEU:HD23	0.44	1.89	15	1
1:A:10:TYR:HB3	1:A:84:HIS:NE2	0.44	2.28	20	1
1:A:38:LYS:HE3	1:A:38:LYS:HA	0.43	1.88	14	1
1:A:13:LEU:HB2	1:A:83:LEU:HD11	0.43	1.89	13	3
1:A:67:PHE:CD1	1:A:67:PHE:N	0.42	2.88	15	2
1:A:93:LYS:HD3	1:A:93:LYS:H	0.42	1.74	6	1
1:A:13:LEU:O	1:A:17:GLN:HG2	0.42	2.15	1	1
1:A:18:LYS:HE2	1:A:18:LYS:HA	0.41	1.92	16	1
1:A:83:LEU:HD12	1:A:88:ARG:HB3	0.41	1.93	15	2
1:A:62:PHE:HE1	1:A:72:ARG:HA	0.41	1.75	2	1
1:A:43:TRP:HB2	1:A:67:PHE:CD1	0.41	2.50	13	1
1:A:53:GLN:NE2	1:A:61:ASN:ND2	0.41	2.69	7	1
1:A:40:LEU:HB3	1:A:50:LEU:HD21	0.41	1.92	19	1
1:A:72:ARG:O	1:A:76:LYS:HG2	0.41	2.16	20	1
1:A:83:LEU:HD13	1:A:84:HIS:N	0.40	2.31	7	2
1:A:13:LEU:HD23	1:A:91:ILE:HB	0.40	1.93	11	1
1:A:88:ARG:O	1:A:92:ALA:HB2	0.40	2.16	19	1
1:A:61:ASN:O	1:A:65:VAL:HG22	0.40	2.15	8	1
1:A:93:LYS:N	1:A:93:LYS:HD2	0.40	2.31	14	1
1:A:36:LEU:O	1:A:36:LEU:HD13	0.40	2.16	19	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	95/98 (97%)	79±2 (84±3%)	13±3 (14±3%)	3±1 (3±1%)	6	41
All	All	1900/1960 (97%)	1589 (84%)	260 (14%)	51 (3%)	6	41

All 7 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	30	HIS	20
1	A	43	TRP	16
1	A	68	SER	11
1	A	56	GLY	1
1	A	8	VAL	1
1	A	19	HIS	1
1	A	42	GLU	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	86/87 (99%)	78±2 (91±2%)	8±2 (9±2%)	11	56
All	All	1720/1740 (99%)	1560 (91%)	160 (9%)	11	56

All 28 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	83	LEU	19
1	A	36	LEU	18
1	A	23	LYS	17
1	A	38	LYS	16
1	A	47	GLU	16
1	A	50	LEU	13
1	A	67	PHE	10
1	A	93	LYS	7
1	A	53	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	62	PHE	6
1	A	20	LYS	4
1	A	96	GLU	4
1	A	51	ARG	3
1	A	6	LYS	2
1	A	82	GLU	2
1	A	90	LYS	2
1	A	17	GLN	2
1	A	77	LYS	2
1	A	98	LEU	2
1	A	14	GLU	1
1	A	91	ILE	1
1	A	76	LYS	1
1	A	61	ASN	1
1	A	73	GLU	1
1	A	87	ASP	1
1	A	18	LYS	1
1	A	41	GLU	1
1	A	72	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping [i](#)

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	920
Number of shifts mapped to atoms	920
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	91	-0.27 ± 0.32	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	0.17 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	83	0.04 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 68%, i.e. 899 atoms were assigned a chemical shift out of a possible 1314. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	364/480 (76%)	190/195 (97%)	91/192 (47%)	83/93 (89%)
Sidechain	492/712 (69%)	387/455 (85%)	105/233 (45%)	0/24 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	43/122 (35%)	42/59 (71%)	0/53 (0%)	1/10 (10%)
Overall	899/1314 (68%)	619/709 (87%)	196/478 (41%)	84/127 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 899 atoms were assigned a chemical shift out of a possible 1335. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	364/490 (74%)	190/199 (95%)	91/196 (46%)	83/95 (87%)
Sidechain	492/723 (68%)	387/462 (84%)	105/237 (44%)	0/24 (0%)
Aromatic	43/122 (35%)	42/59 (71%)	0/53 (0%)	1/10 (10%)
Overall	899/1335 (67%)	619/720 (86%)	196/486 (40%)	84/129 (65%)

7.1.4 Statistically unusual chemical shifts ⓘ

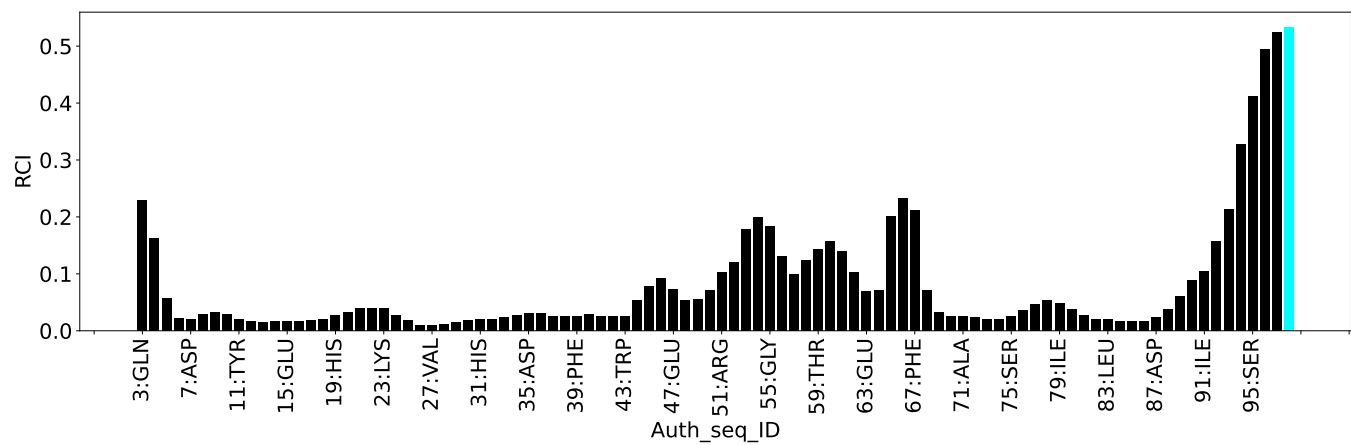
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	37	THR	HG1	6.25	0.08 – 2.19	24.2
1	A	59	THR	HG1	5.04	0.08 – 2.19	18.5
1	A	12	THR	HG1	4.92	0.08 – 2.19	17.9
1	A	69	THR	HG1	4.91	0.08 – 2.19	17.9
1	A	25	THR	HG1	4.42	0.08 – 2.19	15.5
1	A	80	ILE	HD11	-0.93	-0.72 – 2.09	-5.7
1	A	80	ILE	HD12	-0.93	-0.72 – 2.09	-5.7
1	A	80	ILE	HD13	-0.93	-0.72 – 2.09	-5.7
1	A	86	ASP	H	11.27	5.52 – 11.08	5.3

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	1249
Intra-residue ($ i-j =0$)	243
Sequential ($ i-j =1$)	326
Medium range ($ i-j >1$ and $ i-j <5$)	290
Long range ($ i-j \geq 5$)	354
Inter-chain	0
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	179
Number of unmapped restraints	0
Number of restraints per residue	14.6
Number of long range restraints per residue ¹	3.8

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)	79.8	0.2
0.2-0.5 (Medium)	172.4	0.5
>0.5 (Large)	46.7	1.0

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)	13.4	4.95
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

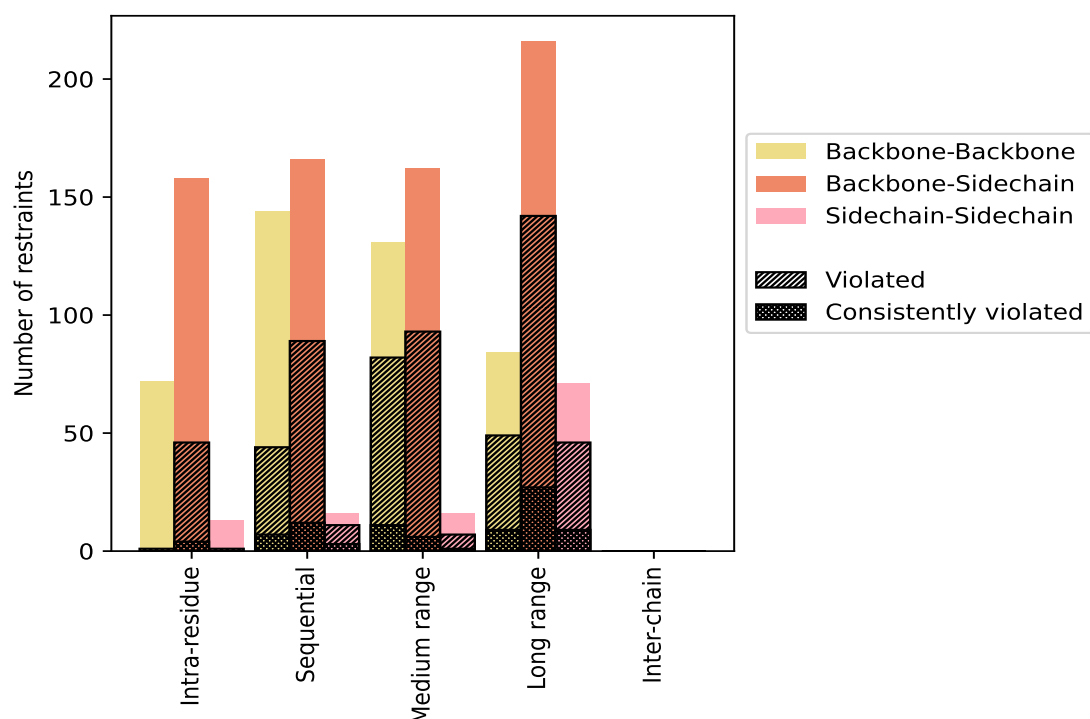
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	243	19.5	48	19.8	3.8	4	1.6	0.3
Backbone-Backbone	72	5.8	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	158	12.7	46	29.1	3.7	4	2.5	0.3
Sidechain-Sidechain	13	1.0	1	7.7	0.1	0	0.0	0.0
Sequential ($i-j =1$)	326	26.1	144	44.2	11.5	22	6.7	1.8
Backbone-Backbone	144	11.5	44	30.6	3.5	7	4.9	0.6
Backbone-Sidechain	166	13.3	89	53.6	7.1	12	7.2	1.0
Sidechain-Sidechain	16	1.3	11	68.8	0.9	3	18.8	0.2
Medium range ($i-j >1$ & $i-j <5$)	290	23.2	174	60.0	13.9	18	6.2	1.4
Backbone-Backbone	131	10.5	82	62.6	6.6	11	8.4	0.9
Backbone-Sidechain	143	11.4	85	59.4	6.8	6	4.2	0.5
Sidechain-Sidechain	16	1.3	7	43.8	0.6	1	6.2	0.1
Long range ($i-j \geq 5$)	354	28.3	231	65.3	18.5	45	12.7	3.6
Backbone-Backbone	84	6.7	49	58.3	3.9	9	10.7	0.7
Backbone-Sidechain	199	15.9	136	68.3	10.9	27	13.6	2.2
Sidechain-Sidechain	71	5.7	46	64.8	3.7	9	12.7	0.7
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	36	2.9	14	38.9	1.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1249	100.0	611	48.9	48.9	89	7.1	7.1
Backbone-Backbone	431	34.5	176	40.8	14.1	27	6.3	2.2
Backbone-Sidechain	702	56.2	370	52.7	29.6	49	7.0	3.9
Sidechain-Sidechain	116	9.3	65	56.0	5.2	13	11.2	1.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations [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	16	68	90	128	0	302	0.33	0.78	0.16	0.31
2	15	73	89	140	0	317	0.32	0.84	0.15	0.3
3	17	71	94	138	0	320	0.32	0.72	0.15	0.31
4	16	66	81	125	0	288	0.32	0.78	0.15	0.3
5	11	67	81	140	0	299	0.33	0.77	0.16	0.3
6	13	76	91	133	0	313	0.31	0.7	0.15	0.3
7	18	70	89	132	0	309	0.34	0.74	0.16	0.34
8	19	66	79	124	0	288	0.33	0.77	0.16	0.31
9	19	68	85	137	0	309	0.34	0.83	0.17	0.32
10	14	62	89	133	0	298	0.33	0.88	0.16	0.31

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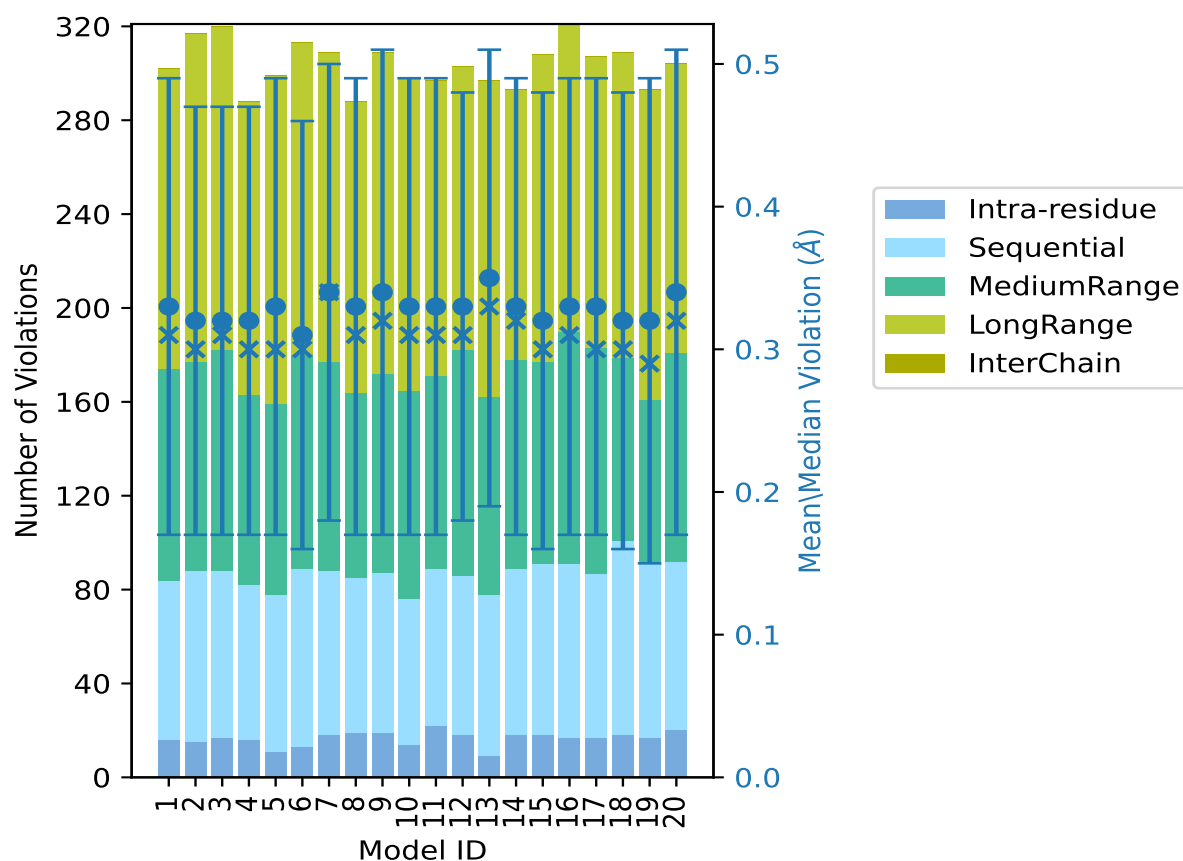
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	22	67	82	126	0	297	0.33	0.72	0.16	0.31
12	18	68	96	121	0	303	0.33	0.75	0.15	0.31
13	9	69	84	135	0	297	0.35	0.91	0.16	0.33
14	18	71	89	115	0	293	0.33	0.7	0.16	0.32
15	18	73	86	131	0	308	0.32	0.79	0.16	0.3
16	17	74	99	131	0	321	0.33	0.79	0.16	0.31
17	17	70	96	124	0	307	0.33	0.69	0.16	0.3
18	18	83	78	130	0	309	0.32	0.78	0.16	0.3
19	17	74	70	132	0	293	0.32	0.76	0.17	0.29
20	20	72	89	123	0	304	0.34	1.0	0.17	0.32

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

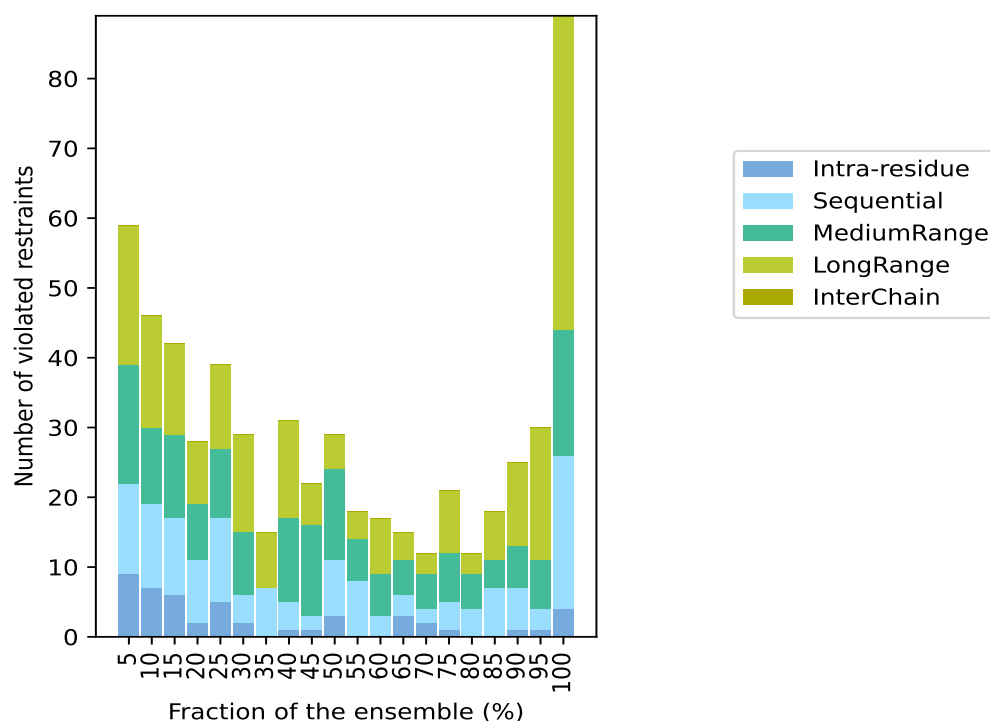
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 616(IR:195, SQ:182, MR:116, LR:123, IC:0) restraints are 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	%
9	13	17	20	0	59	1	5.0
7	12	11	16	0	46	2	10.0
6	11	12	13	0	42	3	15.0
2	9	8	9	0	28	4	20.0
5	12	10	12	0	39	5	25.0
2	4	9	14	0	29	6	30.0
0	7	0	8	0	15	7	35.0
1	4	12	14	0	31	8	40.0
1	2	13	6	0	22	9	45.0
3	8	13	5	0	29	10	50.0
0	8	6	4	0	18	11	55.0
0	3	6	8	0	17	12	60.0
3	3	5	4	0	15	13	65.0
2	2	5	3	0	12	14	70.0
1	4	7	9	0	21	15	75.0
0	4	5	3	0	12	16	80.0
0	7	4	7	0	18	17	85.0
1	6	6	12	0	25	18	90.0
1	3	7	19	0	30	19	95.0
4	22	18	45	0	89	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

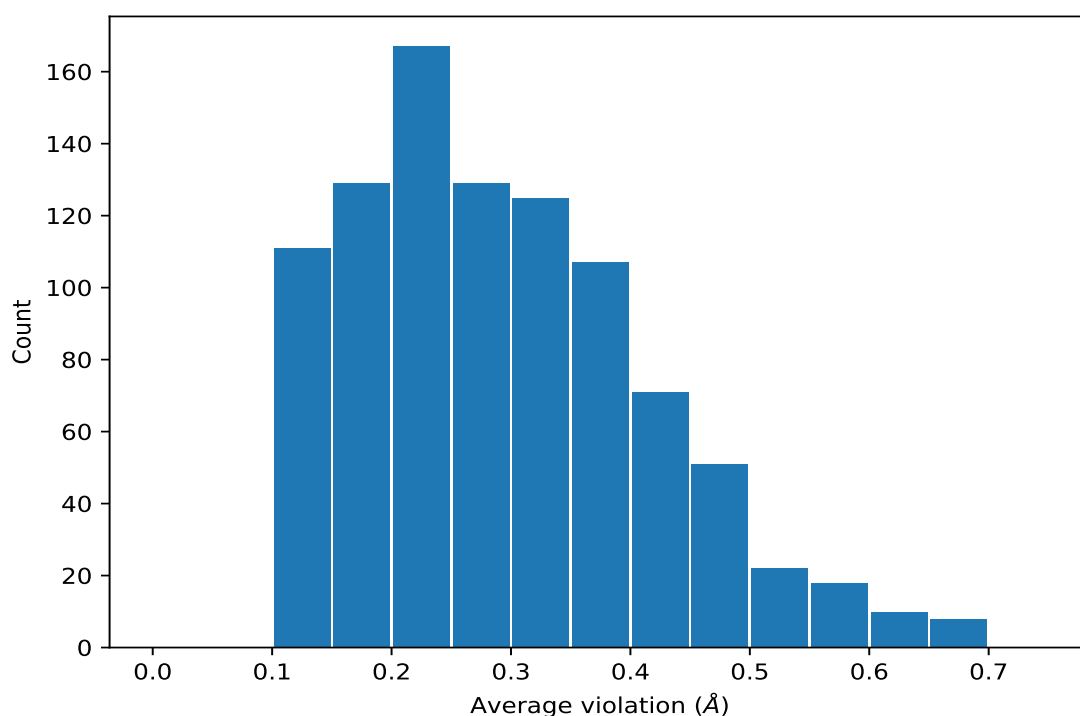
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	20	0.66	0.06	0.68
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	20	0.66	0.06	0.68
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	20	0.66	0.05	0.68
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	20	0.66	0.05	0.68
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	20	0.62	0.06	0.64
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	20	0.62	0.06	0.64
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	20	0.61	0.06	0.62
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	20	0.61	0.07	0.62
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	20	0.61	0.07	0.62
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	20	0.61	0.07	0.62
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	20	0.55	0.07	0.57
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	20	0.55	0.07	0.57
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	20	0.55	0.07	0.57
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	20	0.55	0.08	0.58
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	20	0.55	0.06	0.55
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	20	0.55	0.09	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	20	0.55	0.12	0.54
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	20	0.55	0.12	0.54
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	20	0.55	0.12	0.54
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	20	0.54	0.15	0.52
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	20	0.53	0.11	0.55
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	20	0.53	0.11	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	20	0.52	0.09	0.54
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	20	0.52	0.09	0.54
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	20	0.52	0.09	0.54
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	20	0.49	0.09	0.46
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	20	0.49	0.09	0.46
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	20	0.49	0.09	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	20	0.49	0.06	0.48
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	20	0.49	0.06	0.48
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	20	0.49	0.06	0.48
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	20	0.49	0.12	0.52
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	20	0.48	0.03	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	20	0.48	0.03	0.48
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	20	0.48	0.03	0.48
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	20	0.47	0.14	0.46
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	20	0.47	0.13	0.45
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	20	0.47	0.16	0.5
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	20	0.47	0.07	0.48
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	20	0.47	0.02	0.46
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	20	0.47	0.02	0.46
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	20	0.47	0.02	0.46
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	20	0.46	0.07	0.45
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	20	0.46	0.12	0.48
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	20	0.46	0.06	0.47
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	20	0.46	0.07	0.48
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	20	0.46	0.04	0.46
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	20	0.46	0.14	0.49
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	20	0.46	0.14	0.49
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	20	0.46	0.09	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	20	0.46	0.09	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	20	0.46	0.09	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	20	0.46	0.09	0.5
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	20	0.46	0.09	0.44
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	20	0.46	0.06	0.47
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	20	0.46	0.03	0.45
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	20	0.44	0.09	0.45
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	20	0.44	0.09	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	20	0.44	0.09	0.45
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	20	0.44	0.08	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	20	0.44	0.08	0.48
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	20	0.44	0.09	0.46
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	20	0.43	0.08	0.43
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	20	0.43	0.1	0.4
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	20	0.43	0.1	0.4
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	20	0.43	0.1	0.4
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	20	0.43	0.1	0.4
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	20	0.43	0.11	0.44
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	20	0.42	0.04	0.44
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	20	0.41	0.09	0.41
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	20	0.41	0.09	0.44
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	20	0.4	0.06	0.42
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	20	0.4	0.06	0.42
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	20	0.4	0.09	0.4
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	20	0.4	0.09	0.4
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	20	0.4	0.09	0.4
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	20	0.4	0.03	0.39
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	20	0.4	0.08	0.38
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	20	0.39	0.12	0.4
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	20	0.39	0.08	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	20	0.39	0.08	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	20	0.39	0.08	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	20	0.39	0.08	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	20	0.39	0.08	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	20	0.39	0.08	0.38
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	20	0.39	0.04	0.38
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	20	0.39	0.04	0.38
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	20	0.39	0.11	0.38
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	20	0.38	0.1	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	20	0.38	0.1	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	20	0.38	0.1	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	20	0.38	0.1	0.43
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	20	0.38	0.02	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	20	0.38	0.07	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	20	0.38	0.07	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	20	0.38	0.07	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	20	0.38	0.07	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	20	0.38	0.07	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	20	0.38	0.07	0.38
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	20	0.37	0.07	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	20	0.37	0.07	0.37
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	20	0.37	0.07	0.37
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	20	0.37	0.09	0.42
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	20	0.37	0.09	0.42
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	20	0.37	0.06	0.36
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	20	0.37	0.06	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	20	0.37	0.07	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	20	0.37	0.07	0.36
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	20	0.36	0.1	0.4
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	20	0.36	0.11	0.36
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	20	0.35	0.08	0.35
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	20	0.35	0.07	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	20	0.35	0.07	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	20	0.35	0.07	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	20	0.35	0.07	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	20	0.35	0.07	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	20	0.35	0.07	0.38
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	20	0.34	0.08	0.36
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	20	0.34	0.06	0.35
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	20	0.34	0.06	0.35
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	20	0.34	0.06	0.35
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	20	0.34	0.03	0.35
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	20	0.34	0.08	0.34
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	20	0.34	0.08	0.34
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	20	0.34	0.08	0.34
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	20	0.34	0.09	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	20	0.34	0.09	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	20	0.34	0.09	0.35
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	20	0.33	0.08	0.34
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	20	0.33	0.08	0.34
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	20	0.33	0.14	0.28
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	20	0.33	0.14	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	20	0.33	0.11	0.32
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	20	0.32	0.09	0.32
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	20	0.32	0.09	0.32
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	20	0.32	0.09	0.32
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	20	0.32	0.07	0.34
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	20	0.32	0.07	0.34
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	20	0.32	0.07	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	20	0.32	0.07	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	20	0.32	0.07	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	20	0.32	0.07	0.34
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	20	0.31	0.07	0.33
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	20	0.31	0.03	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	20	0.31	0.03	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	20	0.31	0.03	0.31
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	20	0.3	0.08	0.33
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	20	0.3	0.08	0.33
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	20	0.3	0.08	0.32
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	20	0.3	0.04	0.31
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	20	0.29	0.11	0.27
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	20	0.28	0.03	0.27
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	20	0.28	0.03	0.27
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	20	0.28	0.03	0.28
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	20	0.28	0.09	0.28
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	20	0.28	0.09	0.28
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	20	0.28	0.09	0.28
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	20	0.26	0.05	0.27
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	20	0.25	0.1	0.22
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	20	0.24	0.09	0.26
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	20	0.24	0.06	0.26
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	20	0.2	0.03	0.21
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	20	0.18	0.04	0.2
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	20	0.13	0.01	0.13
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	19	0.66	0.07	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	19	0.65	0.07	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	19	0.65	0.07	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	19	0.65	0.07	0.67
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	19	0.61	0.11	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	19	0.61	0.11	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	19	0.61	0.11	0.65
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	19	0.53	0.26	0.48
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	19	0.53	0.13	0.55
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	19	0.52	0.1	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	19	0.52	0.12	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	19	0.52	0.12	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	19	0.52	0.12	0.55
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	19	0.5	0.2	0.46
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	19	0.5	0.11	0.52
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	19	0.5	0.11	0.52
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	19	0.5	0.14	0.53
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	19	0.47	0.15	0.53
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	19	0.47	0.15	0.53
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	19	0.45	0.11	0.47
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	19	0.45	0.11	0.47
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	19	0.44	0.09	0.46
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	19	0.43	0.18	0.47
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	19	0.42	0.13	0.42
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	19	0.42	0.13	0.42
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	19	0.4	0.14	0.41
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	19	0.4	0.14	0.41
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	19	0.4	0.11	0.43
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	19	0.4	0.11	0.43
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	19	0.4	0.11	0.43
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	19	0.37	0.11	0.41
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	19	0.37	0.11	0.41
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	19	0.36	0.17	0.38
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	19	0.36	0.17	0.38
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	19	0.36	0.08	0.39
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	19	0.36	0.08	0.39
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	19	0.36	0.08	0.39
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	19	0.36	0.07	0.38
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	19	0.35	0.1	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	19	0.35	0.1	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	19	0.35	0.1	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	19	0.35	0.1	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	19	0.35	0.1	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	19	0.35	0.1	0.39
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	19	0.34	0.07	0.36
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	19	0.32	0.1	0.34
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	19	0.32	0.1	0.34
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	19	0.32	0.1	0.34
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	19	0.28	0.08	0.29
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	19	0.28	0.08	0.27
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	19	0.24	0.08	0.25
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	19	0.23	0.08	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	19	0.21	0.06	0.21
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	19	0.21	0.06	0.21
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	19	0.15	0.02	0.14
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	18	0.54	0.17	0.59
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	18	0.53	0.18	0.59
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	18	0.49	0.12	0.54
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	18	0.44	0.14	0.48
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	18	0.44	0.14	0.48
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	18	0.43	0.16	0.43
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	18	0.42	0.13	0.46
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	18	0.42	0.13	0.46
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	18	0.42	0.13	0.46
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	18	0.41	0.09	0.44
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	18	0.41	0.09	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	18	0.4	0.04	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	18	0.4	0.04	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	18	0.4	0.04	0.41
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	18	0.37	0.13	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	18	0.37	0.13	0.39
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	18	0.36	0.08	0.39
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	18	0.35	0.11	0.36
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	18	0.34	0.1	0.34
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	18	0.34	0.08	0.33
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	18	0.34	0.08	0.33
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	18	0.34	0.15	0.34
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	18	0.34	0.15	0.34
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	18	0.34	0.06	0.32
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	18	0.31	0.1	0.34
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	18	0.31	0.1	0.34
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	18	0.31	0.1	0.34
(1,191)	1:25:A:THR:H	1:37:A:THR:H	18	0.3	0.12	0.33
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	18	0.29	0.1	0.3
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	18	0.29	0.1	0.3
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	18	0.29	0.1	0.3
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	18	0.27	0.07	0.28
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	18	0.26	0.08	0.28
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	18	0.25	0.1	0.24
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	18	0.25	0.08	0.26
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	18	0.25	0.07	0.25
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	18	0.21	0.07	0.19
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	18	0.15	0.02	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	18	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	18	0.15	0.02	0.15
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	17	0.43	0.15	0.41
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	17	0.43	0.22	0.4
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	17	0.37	0.1	0.37
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	17	0.36	0.12	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	17	0.35	0.09	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	17	0.35	0.09	0.36
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	17	0.33	0.14	0.28
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	17	0.32	0.09	0.3
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	17	0.32	0.09	0.3
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	17	0.32	0.09	0.3
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	17	0.3	0.12	0.29
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	17	0.29	0.11	0.3
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	17	0.29	0.11	0.3
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	17	0.29	0.11	0.3
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	17	0.29	0.11	0.23
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	17	0.28	0.1	0.28
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	17	0.26	0.08	0.24
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	17	0.26	0.08	0.24
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	17	0.25	0.08	0.24
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	17	0.23	0.06	0.23
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	17	0.23	0.09	0.2
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	17	0.22	0.06	0.22
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	17	0.2	0.05	0.19
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	17	0.2	0.05	0.19
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	17	0.12	0.01	0.12
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	16	0.57	0.09	0.6
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	16	0.47	0.13	0.5
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	16	0.47	0.13	0.5
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	16	0.35	0.17	0.33
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	16	0.34	0.17	0.3
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	16	0.31	0.09	0.31
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	16	0.27	0.1	0.23
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	16	0.24	0.07	0.26
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	16	0.24	0.07	0.26
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	16	0.24	0.07	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	16	0.24	0.07	0.22
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	16	0.22	0.08	0.22
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	16	0.2	0.05	0.2
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	16	0.2	0.05	0.2
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	16	0.2	0.05	0.2
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	16	0.2	0.07	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	16	0.17	0.05	0.16
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	15	0.56	0.22	0.65
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	15	0.41	0.16	0.41
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	15	0.39	0.1	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	15	0.39	0.1	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	15	0.39	0.1	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	15	0.39	0.1	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	15	0.39	0.1	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	15	0.39	0.1	0.42
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	15	0.37	0.16	0.4
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	15	0.37	0.16	0.4
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	15	0.37	0.16	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	15	0.37	0.16	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	15	0.37	0.16	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	15	0.37	0.16	0.4
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	15	0.34	0.08	0.37
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	15	0.31	0.12	0.27
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	15	0.31	0.13	0.35
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	15	0.31	0.13	0.35
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	15	0.31	0.13	0.35
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	15	0.3	0.08	0.32
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	15	0.29	0.12	0.27
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	15	0.27	0.05	0.28
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	15	0.25	0.09	0.22
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	15	0.25	0.12	0.22
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	15	0.25	0.12	0.22
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	15	0.25	0.12	0.22
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	15	0.24	0.07	0.27
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	15	0.23	0.05	0.23
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	15	0.21	0.07	0.2
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	15	0.21	0.05	0.22
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	15	0.2	0.07	0.19
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	15	0.19	0.04	0.2
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	15	0.18	0.05	0.18
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	15	0.14	0.02	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	15	0.14	0.02	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	15	0.14	0.02	0.14
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	15	0.14	0.03	0.14
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	15	0.12	0.01	0.13
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	14	0.5	0.15	0.55
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	14	0.43	0.19	0.41
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	14	0.35	0.11	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	14	0.35	0.11	0.33
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	14	0.35	0.11	0.33
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	14	0.34	0.16	0.39
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	14	0.34	0.16	0.39
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	14	0.31	0.06	0.32
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	14	0.31	0.06	0.32
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	14	0.31	0.06	0.32
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	14	0.28	0.11	0.26
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	14	0.26	0.09	0.26
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	14	0.26	0.07	0.29
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	14	0.25	0.08	0.26
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	14	0.25	0.08	0.26
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	14	0.25	0.08	0.26
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	14	0.25	0.03	0.26
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	14	0.21	0.04	0.2
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	14	0.21	0.04	0.2
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	14	0.21	0.04	0.2
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	14	0.13	0.02	0.14
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	13	0.39	0.18	0.33
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	13	0.39	0.18	0.33
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	13	0.37	0.16	0.38
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	13	0.35	0.13	0.33
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	13	0.35	0.13	0.33
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	13	0.33	0.14	0.3
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	13	0.32	0.12	0.36
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	13	0.3	0.12	0.29
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	13	0.28	0.07	0.26
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	13	0.25	0.07	0.23
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	13	0.21	0.06	0.2
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	13	0.21	0.06	0.2
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	13	0.18	0.07	0.15
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	13	0.18	0.07	0.15
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	13	0.18	0.04	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	13	0.18	0.04	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	13	0.18	0.04	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	13	0.18	0.04	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	13	0.18	0.04	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	13	0.18	0.04	0.17
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	13	0.17	0.04	0.18
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	13	0.17	0.04	0.18
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	13	0.17	0.04	0.18
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	13	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	13	0.16	0.04	0.15
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	13	0.16	0.04	0.15
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	13	0.14	0.03	0.14
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	13	0.13	0.02	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	13	0.13	0.02	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	13	0.13	0.02	0.13
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	12	0.49	0.11	0.5
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	12	0.46	0.14	0.5
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	12	0.44	0.19	0.46
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	12	0.43	0.11	0.44
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	12	0.41	0.09	0.42
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	12	0.36	0.16	0.33
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	12	0.32	0.1	0.35
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	12	0.29	0.07	0.28
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	12	0.27	0.07	0.29
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	12	0.27	0.07	0.28
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	12	0.27	0.09	0.27
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	12	0.25	0.07	0.26
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	12	0.25	0.07	0.26
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	12	0.25	0.07	0.26
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	12	0.24	0.09	0.21
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	12	0.24	0.09	0.21
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	12	0.22	0.09	0.2
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	12	0.22	0.09	0.2
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	12	0.22	0.06	0.22
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	12	0.21	0.05	0.22
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	12	0.21	0.05	0.22
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	12	0.21	0.05	0.22
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	12	0.19	0.06	0.18
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	12	0.19	0.06	0.18
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	12	0.19	0.06	0.18
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	12	0.15	0.05	0.15
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	12	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	12	0.12	0.02	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	12	0.12	0.02	0.12
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	11	0.42	0.13	0.41
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	11	0.4	0.13	0.41
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	11	0.4	0.13	0.41
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	11	0.36	0.15	0.37
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	11	0.35	0.15	0.32
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	11	0.33	0.12	0.37
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	11	0.32	0.1	0.36
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	11	0.29	0.16	0.27
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	11	0.29	0.09	0.29
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	11	0.29	0.09	0.29
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	11	0.29	0.12	0.27
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	11	0.26	0.05	0.27
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	11	0.25	0.11	0.22
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	11	0.25	0.13	0.2
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	11	0.24	0.06	0.26
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	11	0.24	0.06	0.25
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	11	0.24	0.06	0.25
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	11	0.23	0.06	0.24
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	11	0.22	0.07	0.21
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	11	0.22	0.07	0.21
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	11	0.2	0.03	0.21
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	11	0.16	0.05	0.14
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	11	0.12	0.02	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	11	0.12	0.02	0.13
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	10	0.54	0.11	0.56
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	10	0.5	0.12	0.55
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	10	0.5	0.12	0.55
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	10	0.38	0.1	0.36
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	10	0.38	0.1	0.36
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	10	0.38	0.12	0.4
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	10	0.38	0.12	0.4
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	10	0.37	0.16	0.37
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	10	0.37	0.16	0.37
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	10	0.35	0.11	0.33
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	10	0.35	0.08	0.34
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	10	0.33	0.15	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	10	0.33	0.07	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	10	0.33	0.07	0.34
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	10	0.3	0.15	0.3
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	10	0.29	0.1	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	10	0.29	0.09	0.28
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	10	0.27	0.07	0.26
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	10	0.26	0.11	0.24
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	10	0.25	0.07	0.24
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	10	0.24	0.1	0.23
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	10	0.22	0.09	0.24
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	10	0.21	0.05	0.22
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	10	0.21	0.06	0.22
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	10	0.21	0.07	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	10	0.21	0.07	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	10	0.21	0.07	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	10	0.21	0.07	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	10	0.21	0.07	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	10	0.21	0.07	0.18
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	10	0.2	0.08	0.21
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	10	0.2	0.09	0.17
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	10	0.2	0.09	0.17
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	10	0.2	0.05	0.2
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	10	0.18	0.04	0.18
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	10	0.18	0.08	0.18
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	10	0.18	0.06	0.16
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	10	0.17	0.05	0.16
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	10	0.17	0.05	0.16
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	10	0.17	0.05	0.16
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	10	0.13	0.01	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	10	0.11	0.01	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	10	0.11	0.01	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	10	0.11	0.01	0.11
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	9	0.59	0.15	0.64
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	9	0.56	0.09	0.63
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	9	0.56	0.09	0.63
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	9	0.47	0.1	0.48
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	9	0.43	0.2	0.54
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	9	0.41	0.14	0.37
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	9	0.38	0.23	0.25
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	9	0.36	0.13	0.39
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	9	0.34	0.1	0.35
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	9	0.31	0.16	0.23
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	9	0.31	0.1	0.31
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	9	0.31	0.1	0.27
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	9	0.31	0.11	0.33
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	9	0.3	0.16	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	9	0.3	0.16	0.27
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	9	0.29	0.11	0.27
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	9	0.28	0.1	0.31
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	9	0.27	0.13	0.24
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	9	0.27	0.13	0.24
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	9	0.26	0.09	0.25
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	9	0.26	0.09	0.25
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	9	0.21	0.07	0.19
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	9	0.18	0.05	0.17
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	9	0.17	0.05	0.15
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	9	0.17	0.04	0.16
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	9	0.15	0.03	0.13
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	8	0.55	0.13	0.52
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	8	0.55	0.13	0.52
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	8	0.48	0.17	0.45
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	8	0.48	0.17	0.45
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	8	0.47	0.17	0.48
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	8	0.47	0.17	0.48
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	8	0.43	0.11	0.44
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	8	0.43	0.11	0.44
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	8	0.36	0.13	0.35
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	8	0.35	0.12	0.39
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	8	0.35	0.12	0.39
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	8	0.3	0.17	0.24
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	8	0.3	0.17	0.24
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	8	0.3	0.15	0.22
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	8	0.29	0.11	0.3
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	8	0.28	0.11	0.24
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	8	0.28	0.11	0.24
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	8	0.27	0.18	0.18
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	8	0.26	0.13	0.25
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	8	0.25	0.09	0.22
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	8	0.25	0.09	0.22
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	8	0.24	0.08	0.28
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	8	0.24	0.08	0.28
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	8	0.24	0.11	0.21
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	8	0.22	0.08	0.2
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	8	0.22	0.1	0.18
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	8	0.22	0.1	0.18
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	8	0.22	0.08	0.22
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	8	0.22	0.08	0.22
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	8	0.21	0.09	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	8	0.21	0.09	0.18
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	8	0.21	0.07	0.2
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	8	0.21	0.07	0.2
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	8	0.21	0.12	0.16
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	8	0.2	0.07	0.2
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	8	0.2	0.07	0.2
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	8	0.2	0.07	0.2
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	8	0.2	0.07	0.2
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	8	0.2	0.07	0.2
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	8	0.2	0.07	0.2
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	8	0.19	0.04	0.2
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	8	0.19	0.08	0.17
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	8	0.19	0.08	0.17
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	8	0.19	0.08	0.17
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	8	0.18	0.06	0.16
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	8	0.17	0.04	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	8	0.17	0.04	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	8	0.17	0.04	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	8	0.17	0.04	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	8	0.17	0.04	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	8	0.17	0.04	0.15
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	8	0.16	0.05	0.15
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	8	0.16	0.04	0.15
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	8	0.14	0.03	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	8	0.14	0.03	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	8	0.14	0.03	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	8	0.14	0.03	0.14
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	8	0.12	0.02	0.12
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	8	0.11	0.01	0.11
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	7	0.62	0.04	0.63
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	7	0.38	0.17	0.31
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	7	0.34	0.08	0.39
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	7	0.33	0.07	0.31
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	7	0.33	0.07	0.31
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	7	0.32	0.09	0.3
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	7	0.32	0.09	0.3
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	7	0.31	0.2	0.22
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	7	0.31	0.2	0.22
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	7	0.3	0.11	0.28
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	7	0.27	0.08	0.31
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	7	0.27	0.08	0.31
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	7	0.27	0.08	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	7	0.27	0.08	0.31
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	7	0.23	0.08	0.23
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	7	0.21	0.04	0.2
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	7	0.21	0.04	0.2
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	7	0.2	0.1	0.18
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	7	0.2	0.08	0.16
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	7	0.15	0.04	0.14
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	7	0.15	0.02	0.16
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	7	0.15	0.03	0.16
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	7	0.13	0.01	0.13
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	6	0.46	0.16	0.52
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	6	0.46	0.15	0.5
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	6	0.46	0.15	0.5
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	6	0.41	0.23	0.34
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	6	0.36	0.12	0.36
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	6	0.36	0.12	0.36
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	6	0.36	0.08	0.35
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	6	0.36	0.08	0.35
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	6	0.36	0.08	0.35
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	6	0.36	0.08	0.35
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	6	0.33	0.2	0.26
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	6	0.31	0.17	0.24
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	6	0.31	0.17	0.24
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	6	0.31	0.17	0.24
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	6	0.28	0.1	0.31
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	6	0.28	0.1	0.31
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	6	0.27	0.07	0.3
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	6	0.24	0.08	0.22
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	6	0.23	0.12	0.21
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	6	0.22	0.09	0.21
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	6	0.22	0.09	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	6	0.22	0.09	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	6	0.22	0.09	0.21
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	6	0.21	0.06	0.2
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	6	0.2	0.06	0.2
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	6	0.2	0.06	0.2
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	6	0.19	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	6	0.19	0.03	0.18
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	6	0.19	0.03	0.2
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	6	0.19	0.03	0.2
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	6	0.19	0.03	0.2
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	6	0.18	0.06	0.18
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	6	0.17	0.05	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	6	0.17	0.06	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	6	0.17	0.06	0.16
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	6	0.17	0.05	0.14
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	6	0.17	0.05	0.14
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	6	0.16	0.06	0.14
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	6	0.16	0.04	0.16
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	6	0.16	0.02	0.16
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	6	0.15	0.03	0.14
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	6	0.15	0.03	0.14
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	6	0.15	0.04	0.14
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	6	0.14	0.03	0.14
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	6	0.14	0.03	0.14
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	6	0.14	0.03	0.15
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	6	0.14	0.03	0.15
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	6	0.14	0.02	0.14
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	6	0.12	0.01	0.12
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	5	0.6	0.05	0.62
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	5	0.6	0.05	0.62
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	5	0.48	0.11	0.52
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	5	0.48	0.11	0.52
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	5	0.44	0.17	0.48
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	5	0.44	0.17	0.48
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	5	0.42	0.21	0.34
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	5	0.42	0.21	0.34
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	5	0.42	0.21	0.34
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	5	0.41	0.25	0.56
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	5	0.39	0.08	0.41
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	5	0.35	0.19	0.47
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	5	0.35	0.19	0.47
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	5	0.33	0.17	0.27
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	5	0.33	0.15	0.33
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	5	0.33	0.15	0.33
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	5	0.3	0.17	0.28
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	5	0.3	0.11	0.23
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	5	0.3	0.11	0.23
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	5	0.3	0.11	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	5	0.3	0.11	0.23
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	5	0.28	0.06	0.28
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	5	0.28	0.06	0.28
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	5	0.27	0.1	0.24
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	5	0.27	0.08	0.31
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	5	0.27	0.08	0.31
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	5	0.25	0.12	0.3
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	5	0.25	0.12	0.3
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	5	0.25	0.12	0.3
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	5	0.23	0.09	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	5	0.23	0.09	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	5	0.23	0.09	0.18
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	5	0.23	0.14	0.17
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	5	0.23	0.14	0.17
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	5	0.23	0.14	0.17
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	5	0.23	0.06	0.24
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	5	0.21	0.03	0.2
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	5	0.21	0.03	0.2
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	5	0.21	0.1	0.19
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	5	0.2	0.04	0.18
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	5	0.2	0.06	0.24
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	5	0.2	0.08	0.22
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	5	0.2	0.05	0.19
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	5	0.19	0.07	0.15
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	5	0.19	0.07	0.15
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	5	0.18	0.06	0.16
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	5	0.18	0.04	0.18
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	5	0.18	0.04	0.18
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	5	0.18	0.04	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	5	0.18	0.04	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	5	0.18	0.04	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	5	0.18	0.04	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	5	0.18	0.04	0.18
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	5	0.17	0.04	0.16
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	5	0.16	0.04	0.17
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	5	0.16	0.04	0.17
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	5	0.16	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	5	0.16	0.01	0.16
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	5	0.16	0.01	0.16
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	5	0.16	0.02	0.16
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	5	0.15	0.02	0.14
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	5	0.14	0.03	0.15
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	5	0.13	0.02	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	5	0.12	0.01	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	5	0.12	0.01	0.12
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	5	0.12	0.02	0.13
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	5	0.12	0.02	0.13
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	5	0.12	0.02	0.13
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	5	0.12	0.03	0.11
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	5	0.12	0.01	0.11
(1,1088)	1:61:A:ASN:HD21	1:62:A:PHE:HA	4	0.44	0.13	0.44
(2,88)	1:53:A:GLN:HE22	1:56:A:GLY:HA3	4	0.39	0.15	0.37
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB2	4	0.38	0.11	0.36
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB3	4	0.38	0.11	0.36
(1,263)	1:30:A:HIS:HE1	1:31:A:HIS:H	4	0.38	0.17	0.38
(1,1076)	1:43:A:TRP:HD1	1:74:A:LEU:HG	4	0.37	0.2	0.27
(1,366)	1:26:A:TRP:HD1	1:37:A:THR:H	4	0.35	0.25	0.26
(1,276)	1:30:A:HIS:HD1	1:32:A:LYS:H	4	0.33	0.15	0.34
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG2	4	0.33	0.04	0.34
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG3	4	0.33	0.04	0.34
(1,1081)	1:53:A:GLN:HE22	1:64:A:ASP:HB3	4	0.29	0.14	0.27
(1,780)	1:11:A:TYR:H	1:84:A:HIS:H	4	0.24	0.13	0.2
(1,178)	1:23:A:LYS:HZ1	1:24:A:SER:H	4	0.22	0.02	0.22
(1,178)	1:23:A:LYS:HZ2	1:24:A:SER:H	4	0.22	0.02	0.22
(1,178)	1:23:A:LYS:HZ3	1:24:A:SER:H	4	0.22	0.02	0.22
(3,24)	1:37:A:THR:O	1:41:A:GLU:H	4	0.22	0.11	0.2
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG2	4	0.22	0.05	0.21
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG3	4	0.22	0.05	0.21
(1,388)	1:36:A:LEU:HD21	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,388)	1:36:A:LEU:HD22	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,388)	1:36:A:LEU:HD23	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,388)	1:36:A:LEU:HD11	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,388)	1:36:A:LEU:HD12	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,388)	1:36:A:LEU:HD13	1:39:A:PHE:H	4	0.21	0.04	0.2
(1,233)	1:13:A:LEU:HD11	1:28:A:ILE:H	4	0.2	0.12	0.15
(1,233)	1:13:A:LEU:HD12	1:28:A:ILE:H	4	0.2	0.12	0.15
(1,233)	1:13:A:LEU:HD13	1:28:A:ILE:H	4	0.2	0.12	0.15
(1,233)	1:13:A:LEU:HD21	1:28:A:ILE:H	4	0.2	0.12	0.15
(1,233)	1:13:A:LEU:HD22	1:28:A:ILE:H	4	0.2	0.12	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,233)	1:13:A:LEU:HD23	1:28:A:ILE:H	4	0.2	0.12	0.15
(1,175)	1:21:A:ASP:HA	1:24:A:SER:H	4	0.2	0.03	0.2
(1,721)	1:33:A:VAL:HG21	1:80:A:ILE:H	4	0.2	0.08	0.19
(1,721)	1:33:A:VAL:HG22	1:80:A:ILE:H	4	0.2	0.08	0.19
(1,721)	1:33:A:VAL:HG23	1:80:A:ILE:H	4	0.2	0.08	0.19
(1,577)	1:61:A:ASN:HA	1:64:A:ASP:H	4	0.18	0.07	0.15
(1,520)	1:56:A:GLY:HA3	1:57:A:ASP:H	4	0.17	0.06	0.16
(1,680)	1:75:A:SER:HB2	1:77:A:LYS:H	4	0.16	0.04	0.15
(1,680)	1:75:A:SER:HB3	1:77:A:LYS:H	4	0.16	0.04	0.15
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD2	4	0.16	0.04	0.16
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD3	4	0.16	0.04	0.16
(1,824)	1:84:A:HIS:HA	1:88:A:ARG:H	4	0.15	0.04	0.15
(1,1016)	1:16:A:ILE:HA	1:26:A:TRP:HE3	4	0.15	0.05	0.14
(1,1018)	1:16:A:ILE:HD11	1:26:A:TRP:HE3	4	0.15	0.07	0.11
(1,1018)	1:16:A:ILE:HD12	1:26:A:TRP:HE3	4	0.15	0.07	0.11
(1,1018)	1:16:A:ILE:HD13	1:26:A:TRP:HE3	4	0.15	0.07	0.11
(1,784)	1:13:A:LEU:H	1:84:A:HIS:H	4	0.14	0.04	0.14
(1,542)	1:58:A:ALA:HB1	1:59:A:THR:H	4	0.13	0.04	0.12
(1,542)	1:58:A:ALA:HB2	1:59:A:THR:H	4	0.13	0.04	0.12
(1,542)	1:58:A:ALA:HB3	1:59:A:THR:H	4	0.13	0.04	0.12
(2,58)	1:81:A:GLY:H	1:83:A:LEU:H	4	0.13	0.02	0.14
(1,280)	1:31:A:HIS:HB2	1:32:A:LYS:H	4	0.13	0.01	0.13
(1,62)	1:11:A:TYR:HB2	1:12:A:THR:H	4	0.11	0.0	0.11
(1,62)	1:11:A:TYR:HB3	1:12:A:THR:H	4	0.11	0.0	0.11
(1,505)	1:53:A:GLN:H	1:61:A:ASN:HD22	3	0.4	0.05	0.43
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD1	3	0.39	0.1	0.43
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD2	3	0.39	0.1	0.43
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD1	3	0.39	0.1	0.43
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD2	3	0.39	0.1	0.43
(1,662)	1:62:A:PHE:HD1	1:76:A:LYS:H	3	0.37	0.19	0.39
(1,662)	1:62:A:PHE:HD2	1:76:A:LYS:H	3	0.37	0.19	0.39
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG2	3	0.37	0.15	0.46
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG3	3	0.37	0.15	0.46
(1,744)	1:9:A:LYS:HB2	1:81:A:GLY:H	3	0.37	0.08	0.4
(1,631)	1:62:A:PHE:HE1	1:72:A:ARG:H	3	0.34	0.12	0.37
(1,631)	1:62:A:PHE:HE2	1:72:A:ARG:H	3	0.34	0.12	0.37
(1,264)	1:30:A:HIS:HD1	1:31:A:HIS:H	3	0.3	0.12	0.27
(1,947)	1:95:A:SER:HA	1:98:A:LEU:H	3	0.28	0.12	0.26
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE2	3	0.26	0.04	0.24
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE3	3	0.26	0.04	0.24
(1,181)	1:23:A:LYS:HD3	1:24:A:SER:H	3	0.26	0.11	0.33
(1,659)	1:75:A:SER:H	1:78:A:TYR:HB2	3	0.26	0.11	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,164)	1:23:A:LYS:H	1:23:A:LYS:HD3	3	0.26	0.05	0.29
(1,171)	1:23:A:LYS:H	1:25:A:THR:HG1	3	0.25	0.08	0.24
(1,431)	1:39:A:PHE:HA	1:43:A:TRP:H	3	0.25	0.12	0.23
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD21	3	0.23	0.03	0.22
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD22	3	0.23	0.03	0.22
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD23	3	0.23	0.03	0.22
(1,221)	1:16:A:ILE:HD11	1:28:A:ILE:H	3	0.23	0.05	0.22
(1,221)	1:16:A:ILE:HD12	1:28:A:ILE:H	3	0.23	0.05	0.22
(1,221)	1:16:A:ILE:HD13	1:28:A:ILE:H	3	0.23	0.05	0.22
(1,1060)	1:39:A:PHE:HD1	1:75:A:SER:HA	3	0.22	0.14	0.14
(1,1060)	1:39:A:PHE:HD2	1:75:A:SER:HA	3	0.22	0.14	0.14
(1,137)	1:20:A:LYS:HD2	1:21:A:ASP:H	3	0.21	0.08	0.18
(1,137)	1:20:A:LYS:HD3	1:21:A:ASP:H	3	0.21	0.08	0.18
(1,630)	1:39:A:PHE:HZ	1:72:A:ARG:H	3	0.21	0.11	0.15
(1,779)	1:10:A:TYR:HA	1:84:A:HIS:H	3	0.2	0.07	0.17
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD11	3	0.2	0.09	0.15
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD12	3	0.2	0.09	0.15
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD13	3	0.2	0.09	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD11	3	0.2	0.09	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD12	3	0.2	0.09	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD13	3	0.2	0.09	0.15
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA2	3	0.19	0.03	0.21
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA3	3	0.19	0.03	0.21
(1,607)	1:65:A:VAL:HG21	1:67:A:PHE:H	3	0.19	0.03	0.19
(1,607)	1:65:A:VAL:HG22	1:67:A:PHE:H	3	0.19	0.03	0.19
(1,607)	1:65:A:VAL:HG23	1:67:A:PHE:H	3	0.19	0.03	0.19
(1,930)	1:96:A:GLU:H	1:97:A:THR:HA	3	0.19	0.03	0.2
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG2	3	0.18	0.08	0.14
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG3	3	0.18	0.08	0.14
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE1	3	0.18	0.04	0.18
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE2	3	0.18	0.04	0.18
(1,765)	1:10:A:TYR:HA	1:83:A:LEU:H	3	0.18	0.06	0.21
(1,322)	1:34:A:TYR:HB3	1:35:A:ASP:H	3	0.16	0.02	0.16
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD1	3	0.16	0.04	0.16
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD2	3	0.16	0.04	0.16
(1,12)	1:4:A:SER:H	1:6:A:LYS:H	3	0.16	0.06	0.13
(1,434)	1:40:A:LEU:HB2	1:43:A:TRP:H	3	0.16	0.04	0.17
(1,434)	1:40:A:LEU:HB3	1:43:A:TRP:H	3	0.16	0.04	0.17
(1,152)	1:22:A:SER:H	1:23:A:LYS:H	3	0.15	0.0	0.15
(1,318)	1:33:A:VAL:HG21	1:34:A:TYR:H	3	0.14	0.02	0.13
(1,318)	1:33:A:VAL:HG22	1:34:A:TYR:H	3	0.14	0.02	0.13
(1,318)	1:33:A:VAL:HG23	1:34:A:TYR:H	3	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,272)	1:31:A:HIS:H	1:31:A:HIS:HB3	3	0.14	0.02	0.14
(1,432)	1:40:A:LEU:HA	1:43:A:TRP:H	3	0.14	0.01	0.14
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG2	3	0.14	0.02	0.12
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG3	3	0.14	0.02	0.12
(1,451)	1:45:A:GLY:H	1:46:A:GLY:H	3	0.13	0.01	0.13
(1,655)	1:75:A:SER:H	1:75:A:SER:HB2	3	0.13	0.02	0.12
(1,655)	1:75:A:SER:H	1:75:A:SER:HB3	3	0.13	0.02	0.12
(1,1022)	1:25:A:THR:HG21	1:26:A:TRP:HE3	3	0.13	0.02	0.13
(1,1022)	1:25:A:THR:HG22	1:26:A:TRP:HE3	3	0.13	0.02	0.13
(1,1022)	1:25:A:THR:HG23	1:26:A:TRP:HE3	3	0.13	0.02	0.13
(1,158)	1:22:A:SER:H	1:24:A:SER:H	3	0.12	0.01	0.12
(1,855)	1:88:A:ARG:H	1:90:A:LYS:H	3	0.12	0.01	0.13
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD2	3	0.11	0.01	0.11
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD3	3	0.11	0.01	0.11
(2,87)	1:43:A:TRP:HD1	1:67:A:PHE:HB3	2	0.46	0.23	0.46
(1,873)	1:90:A:LYS:HE2	1:91:A:ILE:H	2	0.42	0.03	0.42
(1,873)	1:90:A:LYS:HE3	1:91:A:ILE:H	2	0.42	0.03	0.42
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE1	2	0.42	0.11	0.42
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE2	2	0.42	0.11	0.42
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE1	2	0.42	0.11	0.42
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE2	2	0.42	0.11	0.42
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA2	2	0.38	0.15	0.38
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA3	2	0.38	0.15	0.38
(1,1103)	1:34:A:TYR:HD1	1:75:A:SER:HA	2	0.36	0.07	0.36
(1,1103)	1:34:A:TYR:HD2	1:75:A:SER:HA	2	0.36	0.07	0.36
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE1	2	0.31	0.14	0.31
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE2	2	0.31	0.14	0.31
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE1	2	0.31	0.14	0.31
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE2	2	0.31	0.14	0.31
(1,1113)	1:12:A:THR:HA	1:84:A:HIS:HD2	2	0.31	0.02	0.31
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD1	2	0.3	0.1	0.3
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD2	2	0.3	0.1	0.3
(1,778)	1:84:A:HIS:H	1:84:A:HIS:HD2	2	0.28	0.08	0.28
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE1	2	0.28	0.01	0.28
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE2	2	0.28	0.01	0.28
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG11	2	0.27	0.08	0.27
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG12	2	0.27	0.08	0.27
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG13	2	0.27	0.08	0.27
(1,647)	1:62:A:PHE:HB2	1:75:A:SER:H	2	0.25	0.1	0.25
(2,2)	1:10:A:TYR:H	1:84:A:HIS:HD2	2	0.24	0.13	0.24
(1,174)	1:21:A:ASP:HB2	1:24:A:SER:H	2	0.24	0.06	0.24
(1,174)	1:21:A:ASP:HB3	1:24:A:SER:H	2	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG12	2	0.22	0.12	0.22
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG13	2	0.22	0.12	0.22
(1,741)	1:79:A:ILE:HG21	1:81:A:GLY:H	2	0.22	0.01	0.22
(1,741)	1:79:A:ILE:HG22	1:81:A:GLY:H	2	0.22	0.01	0.22
(1,741)	1:79:A:ILE:HG23	1:81:A:GLY:H	2	0.22	0.01	0.22
(1,562)	1:27:A:VAL:HB	1:62:A:PHE:H	2	0.22	0.04	0.22
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB2	2	0.22	0.08	0.22
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB3	2	0.22	0.08	0.22
(2,66)	1:90:A:LYS:HA	1:93:A:LYS:H	2	0.21	0.09	0.21
(1,858)	1:89:A:SER:HB2	1:90:A:LYS:H	2	0.19	0.0	0.19
(1,858)	1:89:A:SER:HB3	1:90:A:LYS:H	2	0.19	0.0	0.19
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE1	2	0.19	0.08	0.19
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE2	2	0.19	0.08	0.19
(1,563)	1:36:A:LEU:HD21	1:62:A:PHE:H	2	0.18	0.04	0.18
(1,563)	1:36:A:LEU:HD22	1:62:A:PHE:H	2	0.18	0.04	0.18
(1,563)	1:36:A:LEU:HD23	1:62:A:PHE:H	2	0.18	0.04	0.18
(1,336)	1:35:A:ASP:H	1:80:A:ILE:H	2	0.18	0.06	0.18
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG2	2	0.18	0.06	0.18
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG3	2	0.18	0.06	0.18
(1,504)	1:51:A:ARG:HA	1:53:A:GLN:H	2	0.18	0.08	0.18
(1,173)	1:23:A:LYS:HG2	1:24:A:SER:H	2	0.17	0.02	0.17
(1,173)	1:23:A:LYS:HG3	1:24:A:SER:H	2	0.17	0.02	0.17
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD21	2	0.17	0.05	0.17
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD22	2	0.17	0.05	0.17
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD23	2	0.17	0.05	0.17
(1,454)	1:46:A:GLY:H	1:47:A:GLU:H	2	0.17	0.04	0.17
(1,920)	1:94:A:PRO:HG2	1:95:A:SER:H	2	0.17	0.02	0.17
(1,920)	1:94:A:PRO:HG3	1:95:A:SER:H	2	0.17	0.02	0.17
(1,719)	1:34:A:TYR:HB3	1:80:A:ILE:H	2	0.16	0.03	0.16
(1,453)	1:46:A:GLY:H	1:47:A:GLU:HA	2	0.16	0.02	0.16
(1,314)	1:29:A:LEU:HD21	1:34:A:TYR:H	2	0.16	0.04	0.16
(1,314)	1:29:A:LEU:HD22	1:34:A:TYR:H	2	0.16	0.04	0.16
(1,314)	1:29:A:LEU:HD23	1:34:A:TYR:H	2	0.16	0.04	0.16
(1,632)	1:63:A:GLU:HG2	1:72:A:ARG:H	2	0.16	0.01	0.16
(1,632)	1:63:A:GLU:HG3	1:72:A:ARG:H	2	0.16	0.01	0.16
(1,727)	1:78:A:TYR:HA	1:80:A:ILE:H	2	0.15	0.02	0.15
(2,34)	1:53:A:GLN:HE22	1:57:A:ASP:H	2	0.15	0.02	0.15
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD1	2	0.14	0.03	0.14
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD2	2	0.14	0.03	0.14
(1,866)	1:90:A:LYS:H	1:92:A:ALA:HA	2	0.14	0.03	0.14
(1,377)	1:36:A:LEU:HB2	1:38:A:LYS:H	2	0.13	0.03	0.13
(1,377)	1:36:A:LEU:HB3	1:38:A:LYS:H	2	0.13	0.03	0.13

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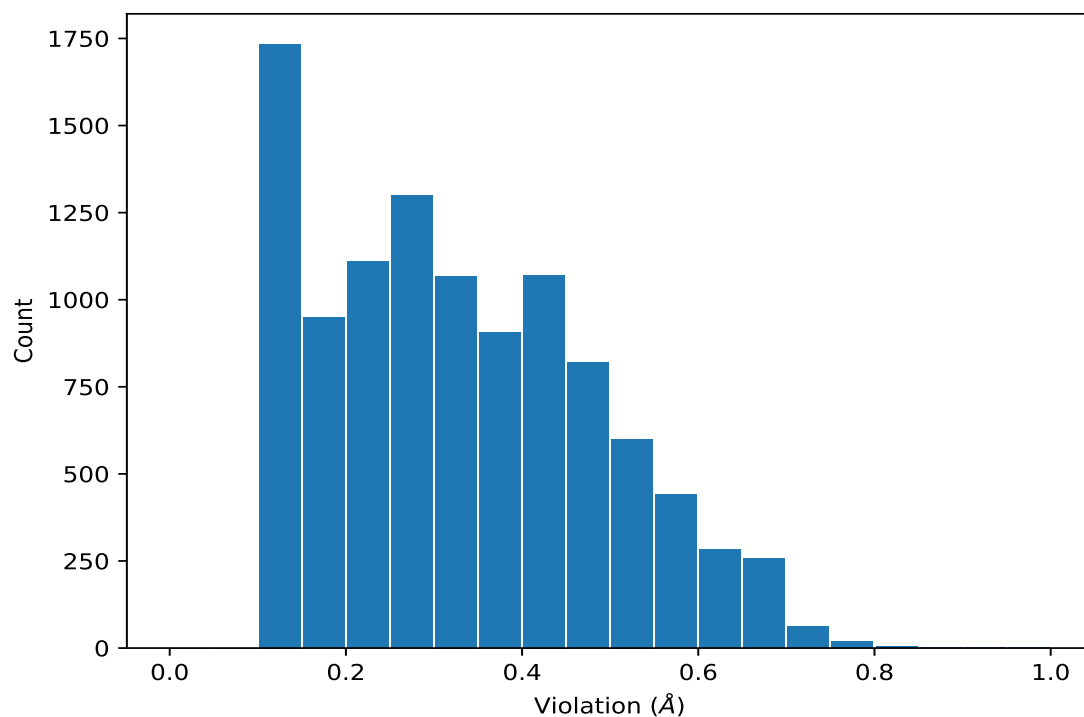
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,510)	1:54:A:ALA:H	1:55:A:GLY:HA3	2	0.13	0.0	0.13
(1,1008)	1:26:A:TRP:HA	1:26:A:TRP:HD1	2	0.13	0.03	0.13
(1,279)	1:31:A:HIS:H	1:32:A:LYS:H	2	0.12	0.02	0.12
(1,917)	1:94:A:PRO:HA	1:95:A:SER:H	2	0.12	0.01	0.12
(1,557)	1:29:A:LEU:HA	1:61:A:ASN:H	2	0.12	0.0	0.12
(1,553)	1:60:A:GLU:HA	1:61:A:ASN:H	2	0.11	0.01	0.11
(1,226)	1:28:A:ILE:H	1:28:A:ILE:HB	2	0.11	0.0	0.11
(1,816)	1:87:A:ASP:H	1:87:A:ASP:HB3	2	0.11	0.0	0.11

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)
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	20	1.0
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	13	0.91
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	10	0.88
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	2	0.84
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	2	0.84
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	2	0.84
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	9	0.83
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	9	0.81
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	15	0.79
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	15	0.79
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	16	0.79
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	18	0.78
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	4	0.78
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	1	0.78
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	8	0.77
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	5	0.77
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	8	0.76
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	5	0.76
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	5	0.76
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	10	0.76
(1,366)	1:26:A:TRP:HD1	1:37:A:THR:H	19	0.76
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	8	0.75
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	8	0.75
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	12	0.75
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	12	0.75
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	12	0.75
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	19	0.75
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	19	0.74
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	19	0.74
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	19	0.74
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	7	0.74
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	10	0.74
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	10	0.74
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	10	0.74
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	5	0.74
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	5	0.74
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	19	0.74
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	4	0.73
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	4	0.73
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	18	0.73
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	13	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	9	0.73
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	20	0.73
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	13	0.72
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	13	0.72
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	7	0.72
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	7	0.72
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	20	0.72
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	20	0.72
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	13	0.72
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	13	0.72
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	20	0.72
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	20	0.72
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	20	0.72
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	3	0.72
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	19	0.72
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	19	0.72
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	19	0.72
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	11	0.72
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	11	0.72
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	11	0.72
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	1	0.71
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	1	0.71
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	18	0.71
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	18	0.71
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	19	0.71
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	19	0.71
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	2	0.71
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	5	0.71
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	18	0.71
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	2	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	1	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	1	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	1	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	16	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	16	0.71
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	16	0.71
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	5	0.71
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	15	0.71
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	20	0.71
(1,1076)	1:43:A:TRP:HD1	1:74:A:LEU:HG	19	0.71
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	13	0.71
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	13	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	9	0.71
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	9	0.71
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	9	0.71
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	3	0.71
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	7	0.71
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	13	0.71
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	20	0.7
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	20	0.7
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	1	0.7
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	1	0.7
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	3	0.7
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	3	0.7
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	9	0.7
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	9	0.7
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	9	0.7
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	3	0.7
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	15	0.7
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	13	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	6	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	6	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	6	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	10	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	10	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	10	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	18	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	18	0.7
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	18	0.7
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	13	0.7
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	8	0.7
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	8	0.7
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	14	0.7
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	14	0.7
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	5	0.7
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	5	0.7
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	15	0.7
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	15	0.7
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	11	0.7
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	20	0.7
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	20	0.7
(2,87)	1:43:A:TRP:HD1	1:67:A:PHE:HB3	9	0.69
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	15	0.69
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	15	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	16	0.69
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	16	0.69
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	9	0.69
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	16	0.69
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	15	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	11	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	11	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	11	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	15	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	15	0.69
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	15	0.69
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	10	0.69
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	7	0.69
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	7	0.69
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	9	0.69
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	9	0.69
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	12	0.69
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	12	0.69
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	13	0.69
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	13	0.69
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	19	0.69
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	16	0.69
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	16	0.69
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	20	0.69
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	17	0.69
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	11	0.68
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	11	0.68
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	11	0.68
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	7	0.68
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	7	0.68
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	17	0.68
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	17	0.68
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	11	0.68
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	11	0.68
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	14	0.68
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	19	0.68
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	8	0.68
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	1	0.68
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	1	0.68
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	3	0.68
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	7	0.68
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	2	0.68
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	20	0.68
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	20	0.68
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	20	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	2	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	2	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	2	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	6	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	6	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	6	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	7	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	7	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	7	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	20	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	20	0.68
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	20	0.68
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	15	0.68
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	15	0.68
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	20	0.68
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	20	0.68
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	10	0.68
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	20	0.68
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	20	0.68
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	11	0.68
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	11	0.68
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	11	0.68
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	18	0.68
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	11	0.67
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	11	0.67
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	6	0.67
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	6	0.67
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	7	0.67
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	7	0.67
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	17	0.67
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	17	0.67
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	1	0.67
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	4	0.67
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	5	0.67
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	16	0.67
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	20	0.67
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	17	0.67
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	8	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	8	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	8	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	12	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	12	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	12	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	13	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	13	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	13	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	14	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	14	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	14	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	17	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	17	0.67
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	17	0.67
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	7	0.67
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	8	0.67
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	16	0.67
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	17	0.67
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	18	0.67
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	7	0.67
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	6	0.67
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	9	0.67
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	6	0.67
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	6	0.67
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	17	0.67
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	17	0.67
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	4	0.67
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	16	0.67
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	7	0.67
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	5	0.67
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	5	0.67
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	5	0.67
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	14	0.67
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	2	0.67
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	9	0.67
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	11	0.67
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	10	0.66
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	10	0.66
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	16	0.66
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	16	0.66
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	10	0.66
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	9	0.66
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	12	0.66
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	6	0.66
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	2	0.66
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	8	0.66
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	1	0.66
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	2	0.66
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	3	0.66
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	12	0.66
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	12	0.66
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	12	0.66
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	12	0.66
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	7	0.66
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	7	0.66
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	12	0.66
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	12	0.66
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	20	0.66
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	20	0.66
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	1	0.66
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	20	0.66
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	10	0.66
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	10	0.66
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	10	0.66
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	19	0.66
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	19	0.66
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	19	0.66
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	7	0.66
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	13	0.66
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	14	0.66
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	19	0.66
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	20	0.66
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	18	0.66
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	7	0.66
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	19	0.66
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	20	0.66
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	14	0.66
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	15	0.66
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	6	0.65
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	6	0.65
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	4	0.65
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	8	0.65
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	8	0.65
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	10	0.65
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	10	0.65
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	13	0.65
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	13	0.65
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	16	0.65
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	16	0.65
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	16	0.65
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	5	0.65
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	1	0.65
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	6	0.65
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	9	0.65
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	9	0.65
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	16	0.65
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	17	0.65
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	17	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	8	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	8	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	8	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	17	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	17	0.65
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	17	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	1	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	1	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	1	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	3	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	3	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	3	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	5	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	5	0.65
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	5	0.65
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	16	0.65
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	16	0.65
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	16	0.65
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	1	0.65
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	11	0.65
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	4	0.65
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	14	0.65
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	4	0.65
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	4	0.65
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	15	0.65
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	15	0.65
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	14	0.65
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	14	0.65
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	14	0.65
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	2	0.65
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	3	0.65
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	15	0.65
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	19	0.65
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	19	0.65
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	16	0.65
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	5	0.64
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	5	0.64
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	9	0.64
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	9	0.64
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	13	0.64
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	13	0.64
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	13	0.64
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	7	0.64
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	14	0.64
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	11	0.64
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	11	0.64
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	5	0.64
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	20	0.64
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	7	0.64
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	11	0.64
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	11	0.64
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	9	0.64
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	9	0.64
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	9	0.64
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	15	0.64
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	4	0.64
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	13	0.64
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	12	0.64
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	10	0.64
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	10	0.64
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	5	0.64
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	15	0.64
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	13	0.64
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	13	0.64
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	3	0.64
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	17	0.64
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	17	0.64
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	17	0.64
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	17	0.64
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	12	0.64
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	16	0.64
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	8	0.64
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	8	0.64
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	8	0.64
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	3	0.64
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	3	0.64
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	10	0.64
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	14	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	4	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	4	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	4	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	5	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	5	0.64
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	5	0.64
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	20	0.64
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	4	0.64
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	14	0.64
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	9	0.64
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	17	0.64
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	5	0.64
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	5	0.64
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	5	0.64
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	19	0.64
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	5	0.63
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	5	0.63
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	7	0.63
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	7	0.63
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	3	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	5	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	5	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	5	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	13	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	13	0.63
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	13	0.63
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	7	0.63
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	7	0.63
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	15	0.63
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	15	0.63
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	15	0.63
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	18	0.63
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	18	0.63
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	18	0.63
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	14	0.63
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	18	0.63
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	6	0.63
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	9	0.63
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	18	0.63
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	4	0.63
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	4	0.63
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	16	0.63
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	16	0.63
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	18	0.63
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	18	0.63
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	5	0.63
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	5	0.63
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	15	0.63
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	15	0.63
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	5	0.63
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	5	0.63
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	19	0.63
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	19	0.63
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	9	0.63
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	7	0.63
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	7	0.63
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	7	0.63
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	17	0.63
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	17	0.63
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	4	0.63
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	4	0.63
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	4	0.63
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	13	0.63
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	3	0.63
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	14	0.63
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	20	0.63
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	2	0.63
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	14	0.63
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	8	0.63
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	20	0.63
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	20	0.63
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	7	0.63
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	12	0.63
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	4	0.63
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	10	0.63
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	19	0.63
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	3	0.63
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	13	0.63
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	9	0.63
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	8	0.62
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	8	0.62
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	8	0.62
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	8	0.62
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	8	0.62
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	8	0.62
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	11	0.62
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	11	0.62
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	14	0.62
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	14	0.62
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	20	0.62
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	16	0.62
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	7	0.62
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	7	0.62
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	6	0.62
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	6	0.62
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	20	0.62
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	16	0.62
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	1	0.62
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	14	0.62
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	14	0.62
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	14	0.62
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	19	0.62
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	19	0.62
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	19	0.62
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	11	0.62
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	11	0.62
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	11	0.62
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	13	0.62
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	6	0.62
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	14	0.62
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	3	0.62
(1,1088)	1:61:A:ASN:HD21	1:62:A:PHE:HA	17	0.62
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	16	0.62
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	16	0.62
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	6	0.62
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	3	0.62
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	7	0.62
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	14	0.62
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	14	0.62
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	14	0.62
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	15	0.62
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	15	0.62
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	15	0.62
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	16	0.62
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	16	0.62
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	16	0.62
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	18	0.62
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	18	0.62
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	1	0.62
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	1	0.62
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	7	0.62
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	7	0.62
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	18	0.62
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	18	0.62
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	9	0.62
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	9	0.62
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	9	0.62
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	15	0.62
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	1	0.62
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	1	0.62
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	19	0.62
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	10	0.62
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	11	0.62
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	14	0.62
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	7	0.62
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	7	0.62
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	7	0.62
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	6	0.62
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	10	0.62
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	15	0.62
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	18	0.62
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	1	0.62
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	11	0.62
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	15	0.62
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	1	0.62
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	2	0.61
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	2	0.61
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	9	0.61
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	9	0.61
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	15	0.61
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	15	0.61
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	1	0.61
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	1	0.61
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	1	0.61
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	13	0.61
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	13	0.61
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	17	0.61
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	17	0.61
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	16	0.61
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	2	0.61
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	5	0.61
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	9	0.61
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	3	0.61
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	16	0.61
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	20	0.61
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	1	0.61
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	1	0.61
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	1	0.61
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	5	0.61
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	5	0.61
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	5	0.61
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	20	0.61
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	11	0.61
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	14	0.61
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	19	0.61
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	16	0.61
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	16	0.61
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	1	0.61
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	1	0.61
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	10	0.61
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	10	0.61
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	11	0.61
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	11	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	14	0.61
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	14	0.61
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	2	0.61
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	2	0.61
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	10	0.61
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	10	0.61
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	3	0.61
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	12	0.61
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	7	0.61
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	7	0.61
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	18	0.61
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	10	0.61
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	14	0.61
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	15	0.61
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	1	0.61
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	1	0.61
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	1	0.61
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	2	0.61
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	2	0.61
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	2	0.61
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	3	0.61
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	3	0.61
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	3	0.61
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	18	0.61
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	18	0.61
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	18	0.61
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	12	0.61
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	12	0.61
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	18	0.61
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	10	0.61
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	10	0.61
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	10	0.61
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	8	0.61
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	12	0.61
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	18	0.61
(1,263)	1:30:A:HIS:HE1	1:31:A:HIS:H	9	0.61
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	11	0.61
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	1	0.61
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	11	0.61
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	20	0.61
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	11	0.61
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	12	0.6
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	12	0.6
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	12	0.6
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	12	0.6
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	13	0.6
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	13	0.6
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	3	0.6
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	3	0.6
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	14	0.6
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	16	0.6
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	3	0.6
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	3	0.6
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	3	0.6
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	7	0.6
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	7	0.6
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	7	0.6
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	7	0.6
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	7	0.6
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	7	0.6
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	9	0.6
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	9	0.6
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	17	0.6
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	11	0.6
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	11	0.6
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	9	0.6
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	9	0.6
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	11	0.6
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	11	0.6
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	11	0.6
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	17	0.6
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	17	0.6
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	17	0.6
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	3	0.6
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	3	0.6
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	20	0.6
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	20	0.6
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	9	0.6
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	9	0.6
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	19	0.6
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	3	0.6
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	17	0.6
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	17	0.6
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	14	0.6
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	14	0.6
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	14	0.6
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	14	0.6
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	7	0.6
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	7	0.6
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	7	0.6
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	10	0.6
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	13	0.6
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	8	0.6
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	19	0.6
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	19	0.6
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	19	0.6
(2,88)	1:53:A:GLN:HE22	1:56:A:GLY:HA3	13	0.59
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	1	0.59
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	14	0.59
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	20	0.59
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	20	0.59
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	2	0.59
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	2	0.59
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	2	0.59
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	15	0.59
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	14	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	2	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	2	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	2	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	16	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	16	0.59
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	16	0.59
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	8	0.59
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	5	0.59
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	5	0.59
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	7	0.59
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	8	0.59
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	3	0.59
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	3	0.59
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	8	0.59
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	8	0.59
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	8	0.59
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	10	0.59
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	9	0.59
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	9	0.59
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	9	0.59
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	9	0.59
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	11	0.59
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	11	0.59
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	11	0.59
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	11	0.59
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	4	0.59
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	4	0.59
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	7	0.59
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	7	0.59
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	4	0.59
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	14	0.59
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	13	0.59
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	13	0.59
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	18	0.59
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	13	0.59
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	13	0.59
(1,662)	1:62:A:PHE:HD1	1:76:A:LYS:H	13	0.59
(1,662)	1:62:A:PHE:HD2	1:76:A:LYS:H	13	0.59
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	7	0.59
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	7	0.59
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	7	0.59
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	2	0.59
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	7	0.59
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	20	0.59
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	6	0.59
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	6	0.59
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	6	0.59
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	10	0.59
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	10	0.59
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	10	0.59
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	10	0.59
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	5	0.59
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	9	0.59
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	15	0.59
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	17	0.59
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	9	0.59
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	19	0.59
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	14	0.58
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	14	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	4	0.58
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	10	0.58
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	8	0.58
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	8	0.58
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	8	0.58
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	6	0.58
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	2	0.58
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	2	0.58
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	12	0.58
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	12	0.58
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	5	0.58
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	5	0.58
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	5	0.58
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	5	0.58
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	2	0.58
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	2	0.58
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	19	0.58
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	19	0.58
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	17	0.58
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	5	0.58
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	15	0.58
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	9	0.58
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	9	0.58
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	6	0.58
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	6	0.58
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	6	0.58
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	20	0.58
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	20	0.58
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	20	0.58
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	10	0.58
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	10	0.58
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	17	0.58
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	17	0.58
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	15	0.58
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	15	0.58
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	8	0.58
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	8	0.58
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	8	0.58
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	3	0.58
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	5	0.58
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	5	0.58
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	14	0.58
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	4	0.58
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	15	0.58
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	11	0.58
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	17	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	7	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	7	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	7	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	17	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	17	0.58
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	17	0.58
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	16	0.58
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	16	0.58
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	16	0.58
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	1	0.58
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	5	0.58
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	13	0.58
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	4	0.58
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	3	0.58
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	3	0.58
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	9	0.58
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	9	0.58
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	17	0.58
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	19	0.57
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	19	0.57
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	4	0.57
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	4	0.57
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	4	0.57
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	9	0.57
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	7	0.57
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	7	0.57
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	14	0.57
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	4	0.57
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	4	0.57
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	11	0.57
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	11	0.57
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	11	0.57
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	3	0.57
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	3	0.57
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	3	0.57
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	20	0.57
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	20	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	20	0.57
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	1	0.57
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	8	0.57
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	16	0.57
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	16	0.57
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	1	0.57
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	18	0.57
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	18	0.57
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	17	0.57
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	17	0.57
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	17	0.57
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	3	0.57
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	3	0.57
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	12	0.57
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	12	0.57
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	12	0.57
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	12	0.57
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	19	0.57
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	12	0.57
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	12	0.57
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	10	0.57
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	17	0.57
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	17	0.57
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	2	0.57
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	1	0.57
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	2	0.57
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	2	0.57
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	19	0.57
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	18	0.57
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	1	0.57
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	16	0.57
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	19	0.57
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	19	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	9	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	9	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	9	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	19	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	19	0.57
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	19	0.57
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	2	0.57
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	2	0.57
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	11	0.57
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	11	0.57
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	11	0.57
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	3	0.57
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	2	0.57
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	2	0.57
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	15	0.57
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	15	0.57
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	2	0.57
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	2	0.57
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	13	0.57
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	8	0.57
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	7	0.57
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	14	0.57
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	6	0.57
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	6	0.57
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	6	0.57
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	15	0.57
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	5	0.57
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	20	0.56
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	20	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	18	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	18	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	18	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	20	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	20	0.56
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	20	0.56
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	1	0.56
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	19	0.56
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	20	0.56
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	2	0.56
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	11	0.56
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	12	0.56
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	9	0.56
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	19	0.56
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	4	0.56
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	12	0.56
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	15	0.56
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	15	0.56
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	15	0.56
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	4	0.56
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	4	0.56
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	14	0.56
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	14	0.56
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	14	0.56
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	17	0.56
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	17	0.56
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	17	0.56
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	8	0.56
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	8	0.56
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	10	0.56
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	2	0.56
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	2	0.56
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	8	0.56
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	8	0.56
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	6	0.56
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	6	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	12	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	12	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	12	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	13	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	13	0.56
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	13	0.56
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	20	0.56
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	20	0.56
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	19	0.56
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	13	0.56
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	9	0.56
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	16	0.56
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	20	0.56
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	18	0.56
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	18	0.56
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	19	0.56
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	16	0.56
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	16	0.56
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	16	0.56
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	15	0.56
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	10	0.56
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	3	0.56
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	10	0.56
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	11	0.56
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	16	0.56
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	6	0.56
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	8	0.56
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	9	0.56
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	1	0.56
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	4	0.56
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	12	0.56
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	17	0.56
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	12	0.56
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	12	0.56
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	12	0.56
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	11	0.56
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	12	0.56
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	14	0.56
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	14	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	8	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	8	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	12	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	12	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	17	0.56
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	17	0.56
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	7	0.56
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	13	0.56
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	17	0.56
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	9	0.56
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	9	0.56
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	9	0.56
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	13	0.56
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	13	0.56
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	13	0.56
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	15	0.56
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	15	0.56
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB2	17	0.55
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB3	17	0.55
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	3	0.55
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	3	0.55
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	3	0.55
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	10	0.55
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	14	0.55
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	7	0.55
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	16	0.55
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	3	0.55
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	17	0.55
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	17	0.55
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	4	0.55
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	4	0.55
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	20	0.55
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	20	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	6	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	6	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	6	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	19	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	19	0.55
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	19	0.55
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	9	0.55
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	9	0.55
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	15	0.55
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	15	0.55
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	5	0.55
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	6	0.55
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	4	0.55
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	4	0.55
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	7	0.55
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	13	0.55
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	1	0.55
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	1	0.55
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	14	0.55
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	14	0.55
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	15	0.55
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	18	0.55
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	18	0.55
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	5	0.55
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	8	0.55
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	12	0.55
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	15	0.55
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	8	0.55
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	16	0.55
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	1	0.55
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	6	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	10	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	10	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	10	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	11	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	11	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	11	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	12	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	12	0.55
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	12	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	1	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	1	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	1	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	18	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	18	0.55
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	18	0.55
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	1	0.55
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	16	0.55
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	12	0.55
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	3	0.55
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	18	0.55
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	13	0.55
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	8	0.55
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	4	0.55
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	4	0.55
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	4	0.55
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	17	0.54
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	1	0.54
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	4	0.54
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	8	0.54
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	14	0.54
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	17	0.54
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	17	0.54
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	7	0.54
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	7	0.54
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	17	0.54
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	17	0.54
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	17	0.54
(2,15)	1:24:A:SER:H	1:37:A:THR:HB	6	0.54
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	5	0.54
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	18	0.54
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	13	0.54
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	13	0.54
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	2	0.54
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	12	0.54
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	16	0.54
(1,1054)	1:34:A:TYR:HD1	1:83:A:LEU:HB2	19	0.54
(1,1054)	1:34:A:TYR:HD2	1:83:A:LEU:HB2	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	16	0.54
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	16	0.54
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	1	0.54
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	1	0.54
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	1	0.54
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	5	0.54
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	5	0.54
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	7	0.54
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	7	0.54
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	7	0.54
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	7	0.54
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	14	0.54
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	14	0.54
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	13	0.54
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	17	0.54
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	20	0.54
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	7	0.54
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	9	0.54
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	11	0.54
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	12	0.54
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	9	0.54
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	10	0.54
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	2	0.54
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	2	0.54
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	6	0.54
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	6	0.54
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	10	0.54
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	10	0.54
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	16	0.54
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	16	0.54
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	1	0.54
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	1	0.54
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	13	0.54
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	13	0.54
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	6	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	11	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	11	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	11	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	11	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	11	0.54
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	11	0.54
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	10	0.54
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	15	0.54
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	8	0.54
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	8	0.54
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	14	0.54
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	14	0.54
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	4	0.54
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	6	0.54
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	11	0.54
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	14	0.54
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	19	0.54
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	11	0.54
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	2	0.54
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	2	0.54
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	2	0.54
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	6	0.54
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	13	0.54
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	9	0.54
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	8	0.54
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	15	0.54
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	7	0.54
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	12	0.54
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	13	0.54
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	13	0.54
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	18	0.54
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	18	0.54
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	6	0.54
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	7	0.54
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	9	0.54
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	15	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	12	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	12	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	12	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	17	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	17	0.54
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	17	0.54
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	12	0.53
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	12	0.53
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	12	0.53
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	12	0.53
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	12	0.53
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	12	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	14	0.53
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	14	0.53
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	5	0.53
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	5	0.53
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	5	0.53
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	7	0.53
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	16	0.53
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	11	0.53
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	11	0.53
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	17	0.53
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	8	0.53
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	8	0.53
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	20	0.53
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	17	0.53
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	13	0.53
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	15	0.53
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	15	0.53
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	15	0.53
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	9	0.53
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	9	0.53
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	9	0.53
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	15	0.53
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	15	0.53
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE1	3	0.53
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE2	3	0.53
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE1	3	0.53
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE2	3	0.53
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	17	0.53
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	18	0.53
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	18	0.53
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	8	0.53
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	8	0.53
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	17	0.53
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	17	0.53
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	11	0.53
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	11	0.53
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	8	0.53
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	8	0.53
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	7	0.53
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	11	0.53
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	4	0.53
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	13	0.53
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	13	0.53
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	13	0.53
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	7	0.53
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	5	0.53
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	5	0.53
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	7	0.53
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	7	0.53
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	18	0.53
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	18	0.53
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	14	0.53
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	14	0.53
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	5	0.53
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	5	0.53
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	5	0.53
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	10	0.53
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	10	0.53
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	10	0.53
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	15	0.53
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	18	0.53
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	6	0.53
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	6	0.53
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	9	0.53
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	20	0.53
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	20	0.53
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	20	0.53
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	6	0.53
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	9	0.53
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	8	0.53
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	5	0.53
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	12	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	3	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	3	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	3	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	6	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	6	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	6	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	15	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	15	0.53
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	15	0.53
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	8	0.53
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	8	0.53
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	15	0.53
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	15	0.53
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	15	0.53
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	6	0.53
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	14	0.53
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	14	0.53
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	14	0.53
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	5	0.53
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	5	0.53
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	7	0.53
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	7	0.53
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	14	0.53
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	3	0.53
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	8	0.53
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	4	0.53
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	4	0.53
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	7	0.53
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	7	0.53
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	8	0.53
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	8	0.53
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	7	0.53
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	7	0.53
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	7	0.53
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	6	0.53
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	19	0.53
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	19	0.53
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	8	0.53
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	8	0.53
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	8	0.53
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	12	0.53
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	17	0.53
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	1	0.52
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	1	0.52
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	1	0.52
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	1	0.52
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	1	0.52
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	1	0.52
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	17	0.52
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	17	0.52
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	17	0.52
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	17	0.52
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	17	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	15	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	15	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	15	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	17	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	17	0.52
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	17	0.52
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	2	0.52
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	12	0.52
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	19	0.52
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	18	0.52
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	18	0.52
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	2	0.52
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	11	0.52
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	3	0.52
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	8	0.52
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	4	0.52
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	4	0.52
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	4	0.52
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	6	0.52
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	6	0.52
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	19	0.52
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	19	0.52
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	4	0.52
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	4	0.52
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	4	0.52
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	8	0.52
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	8	0.52
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	8	0.52
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	9	0.52
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	9	0.52
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	9	0.52
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	13	0.52
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	13	0.52
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	13	0.52
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA2	19	0.52
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA3	19	0.52
(1,1088)	1:61:A:ASN:HD21	1:62:A:PHE:HA	20	0.52
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	4	0.52
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	4	0.52
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	20	0.52
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	17	0.52
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	17	0.52
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	17	0.52
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	17	0.52
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	17	0.52
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	17	0.52
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	16	0.52
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	16	0.52
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	4	0.52
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	2	0.52
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	15	0.52
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	4	0.52
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	3	0.52
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	18	0.52
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	12	0.52
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	12	0.52
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	2	0.52
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	3	0.52
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	6	0.52
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	14	0.52
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	18	0.52
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	11	0.52
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	18	0.52
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	3	0.52
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	3	0.52
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	3	0.52
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	3	0.52
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	12	0.52
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	12	0.52
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	16	0.52
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	2	0.52
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	2	0.52
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	2	0.52
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	18	0.52
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	20	0.52
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	3	0.52
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	2	0.52
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	2	0.52
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	13	0.52
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	1	0.52
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	1	0.52
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	1	0.52
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	1	0.52
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	8	0.52
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	8	0.52
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	8	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	5	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	5	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	5	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	13	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	13	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	13	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	16	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	16	0.52
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	16	0.52
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	17	0.52
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	1	0.52
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	1	0.52
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	5	0.52
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	5	0.52
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	15	0.52
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	15	0.52
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	11	0.52
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	20	0.52
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	15	0.52
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	1	0.52
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	17	0.52
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	6	0.52
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	20	0.52
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	20	0.52
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	19	0.52
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	19	0.52
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	19	0.52
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	19	0.52
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	10	0.52
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	16	0.52
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	12	0.52
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	7	0.52
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	16	0.52
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	9	0.52
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	9	0.52
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	15	0.52
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	15	0.52
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	15	0.52
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	19	0.52
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	17	0.51
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	13	0.51
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	13	0.51
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	13	0.51
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	13	0.51
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	13	0.51
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	13	0.51
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	2	0.51
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	1	0.51
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	2	0.51
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	18	0.51
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	18	0.51
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	18	0.51
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	9	0.51
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	9	0.51
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	9	0.51
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	15	0.51
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	15	0.51
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	12	0.51
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	12	0.51
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	10	0.51
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	10	0.51
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	10	0.51
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	10	0.51
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	10	0.51
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	10	0.51
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	14	0.51
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	14	0.51
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	14	0.51
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	8	0.51
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	8	0.51
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	1	0.51
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	1	0.51
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	15	0.51
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	16	0.51
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	17	0.51
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	19	0.51
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	5	0.51
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	14	0.51
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	13	0.51
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	13	0.51
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	15	0.51
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	15	0.51
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	17	0.51
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	13	0.51
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	9	0.51
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	9	0.51
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	18	0.51
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	2	0.51
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	2	0.51
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	6	0.51
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	6	0.51
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	8	0.51
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	8	0.51
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	12	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	17	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	17	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	17	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	17	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	17	0.51
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	17	0.51
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	14	0.51
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	6	0.51
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	12	0.51
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	16	0.51
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	16	0.51
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	6	0.51
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	9	0.51
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	16	0.51
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	16	0.51
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	18	0.51
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	18	0.51
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	19	0.51
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	1	0.51
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	6	0.51
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	6	0.51
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	6	0.51
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	18	0.51
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	17	0.51
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	17	0.51
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	19	0.51
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	19	0.51
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	1	0.51
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	16	0.51
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	5	0.51
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	11	0.51
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	17	0.51
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	2	0.51
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	10	0.51
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	18	0.51
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	20	0.51
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	20	0.51
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	20	0.51
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	13	0.51
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	1	0.51
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	5	0.51
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	17	0.51
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	10	0.51
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	5	0.51
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	5	0.51
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	11	0.51
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	11	0.51
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	6	0.5
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	6	0.5
(2,57)	1:32:A:LYS:HB3	1:81:A:GLY:H	6	0.5
(2,52)	1:32:A:LYS:HB3	1:81:A:GLY:H	6	0.5
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	14	0.5
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	14	0.5
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	17	0.5
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	18	0.5
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	6	0.5
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	10	0.5
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	17	0.5
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	11	0.5
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	7	0.5
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	14	0.5
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	14	0.5
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	14	0.5
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	12	0.5
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	7	0.5
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	7	0.5
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	19	0.5
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	19	0.5
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	19	0.5
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	11	0.5
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	10	0.5
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	10	0.5
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	3	0.5
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	3	0.5
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	3	0.5
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	3	0.5
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	3	0.5
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	3	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	7	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	7	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	7	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	18	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	18	0.5
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	18	0.5
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	10	0.5
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	10	0.5
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	1	0.5
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	1	0.5
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	10	0.5
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	10	0.5
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	13	0.5
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	13	0.5
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	13	0.5
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	13	0.5
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	6	0.5
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	6	0.5
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	2	0.5
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	3	0.5
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	8	0.5
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	1	0.5
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	14	0.5
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	14	0.5
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	14	0.5
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	14	0.5
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	16	0.5
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	18	0.5
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	19	0.5
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	10	0.5
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	15	0.5
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	6	0.5
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	11	0.5
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	11	0.5
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	11	0.5
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	12	0.5
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	5	0.5
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	5	0.5
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	13	0.5
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	2	0.5
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	12	0.5
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	15	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	1	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	1	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	1	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	1	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	1	0.5
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	1	0.5
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	11	0.5
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	12	0.5
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	19	0.5
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	8	0.5
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	7	0.5
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	20	0.5
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	4	0.5
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	4	0.5
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	4	0.5
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	14	0.5
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	14	0.5
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	8	0.5
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	8	0.5
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	19	0.5
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	19	0.5
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	10	0.5
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	10	0.5
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	9	0.5
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	4	0.5
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	5	0.5
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	10	0.5
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	5	0.5
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	6	0.5
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	16	0.5
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	17	0.5
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	17	0.5
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	11	0.5
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	11	0.5
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	17	0.5
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	17	0.5
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	4	0.5
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	4	0.5
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	4	0.5
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	18	0.5
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	18	0.5
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	18	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	3	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	4	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	7	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	10	0.5
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	12	0.5
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	1	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	10	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	10	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	10	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	13	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	13	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	13	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	16	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	16	0.5
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	16	0.5
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	4	0.5
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	18	0.49
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	18	0.49
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	18	0.49
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	9	0.49
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	9	0.49
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	9	0.49
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	9	0.49
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	9	0.49
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	9	0.49
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	11	0.49
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	13	0.49
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	4	0.49
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	15	0.49
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	6	0.49
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	19	0.49
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	19	0.49
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	12	0.49
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	12	0.49
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	12	0.49
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	10	0.49
(1,1081)	1:53:A:GLN:HE22	1:64:A:ASP:HB3	2	0.49
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	12	0.49
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	12	0.49
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD1	12	0.49
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD2	12	0.49
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD1	12	0.49
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD2	12	0.49
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	4	0.49
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	4	0.49
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	4	0.49
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	4	0.49
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	4	0.49
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	4	0.49
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	4	0.49
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	6	0.49
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	6	0.49
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	7	0.49
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	7	0.49
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	19	0.49
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	19	0.49
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	13	0.49
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	13	0.49
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	13	0.49
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	13	0.49
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	13	0.49
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	13	0.49
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	13	0.49
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	12	0.49
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	12	0.49
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	3	0.49
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	3	0.49
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	4	0.49
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	4	0.49
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	4	0.49
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	10	0.49
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	10	0.49
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	10	0.49
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	20	0.49
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	20	0.49
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	20	0.49
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	20	0.49
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	20	0.49
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG2	11	0.49
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG3	11	0.49
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	8	0.49
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	8	0.49
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	20	0.49
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	5	0.49
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	15	0.49
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	17	0.49
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	14	0.49
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	3	0.49
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	10	0.49
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	1	0.49
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	1	0.49
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	5	0.49
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	19	0.49
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	9	0.49
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	9	0.49
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	9	0.49
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	17	0.49
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	17	0.49
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	17	0.49
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	20	0.49
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	20	0.49
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	20	0.49
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	9	0.49
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	9	0.49
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	20	0.49
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	20	0.49
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	14	0.49
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	14	0.49
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	5	0.49
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	15	0.49
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	15	0.49
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	1	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	6	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	6	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	6	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	6	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	6	0.49
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	6	0.49
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	8	0.49
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	5	0.49
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	4	0.49
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	12	0.49
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	19	0.49
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	7	0.49
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	7	0.49
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	12	0.49
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	12	0.49
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	1	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	18	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	18	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	18	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	20	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	20	0.49
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	20	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	12	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	12	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	12	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	17	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	17	0.49
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	17	0.49
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	2	0.49
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	2	0.49
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	4	0.49
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	12	0.49
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	12	0.49
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	1	0.49
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	1	0.49
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	13	0.49
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	13	0.49
(1,276)	1:30:A:HIS:HD1	1:32:A:LYS:H	18	0.49
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	8	0.49
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	1	0.49
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	20	0.49
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	4	0.49
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	3	0.49
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	7	0.49
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	16	0.49
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	16	0.49
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	16	0.49
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	8	0.49
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	9	0.49
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	1	0.49
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	17	0.49
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	20	0.49
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	20	0.49
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	20	0.49
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	2	0.49
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	12	0.49
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	16	0.48
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	16	0.48
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	16	0.48
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	16	0.48
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	16	0.48
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	16	0.48
(2,85)	1:39:A:PHE:HE1	1:43:A:TRP:HD1	3	0.48
(2,85)	1:39:A:PHE:HE2	1:43:A:TRP:HD1	3	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	7	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	7	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	7	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	8	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	8	0.48
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	8	0.48
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	5	0.48
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	10	0.48
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	7	0.48
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	10	0.48
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	10	0.48
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	15	0.48
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	15	0.48
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	16	0.48
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	20	0.48
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	20	0.48
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	6	0.48
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	6	0.48
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	6	0.48
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	3	0.48
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	8	0.48
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	8	0.48
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	1	0.48
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	1	0.48
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	1	0.48
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	1	0.48
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	1	0.48
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	1	0.48
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	15	0.48
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	15	0.48
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	11	0.48
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	16	0.48
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	1	0.48
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	4	0.48
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	13	0.48
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	13	0.48
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	13	0.48
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	8	0.48
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	11	0.48
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	1	0.48
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	9	0.48
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	19	0.48
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	8	0.48
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	11	0.48
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	8	0.48
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	8	0.48
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	2	0.48
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	7	0.48
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	13	0.48
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	20	0.48
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	14	0.48
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	16	0.48
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	17	0.48
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	2	0.48
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	13	0.48
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	15	0.48
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	15	0.48
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	15	0.48
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	5	0.48
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	8	0.48
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	14	0.48
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	14	0.48
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	18	0.48
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	18	0.48
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	18	0.48
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	6	0.48
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	6	0.48
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	6	0.48
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	15	0.48
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	9	0.48
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	10	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	20	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	20	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	20	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	20	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	20	0.48
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	20	0.48
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	1	0.48
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	10	0.48
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	20	0.48
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	3	0.48
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	17	0.48
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	17	0.48
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	9	0.48
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	9	0.48
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	9	0.48
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	9	0.48
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	9	0.48
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	9	0.48
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	15	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	10	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	14	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	14	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	17	0.48
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	17	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	7	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	7	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	12	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	12	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	16	0.48
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	16	0.48
(1,289)	1:11:A:TYR:HB3	1:33:A:VAL:H	19	0.48
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	3	0.48
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	16	0.48
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	3	0.48
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	10	0.48
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	10	0.48
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	10	0.48
(1,191)	1:25:A:THR:H	1:37:A:THR:H	9	0.48
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	9	0.48
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	3	0.48
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	10	0.48
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	1	0.48
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	1	0.48
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	12	0.48
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	12	0.48
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	2	0.48
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	2	0.48
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	2	0.48
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	10	0.48
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	10	0.48
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	10	0.48
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	14	0.48
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	14	0.48
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	14	0.48
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	18	0.48
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	20	0.48
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	14	0.48
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	2	0.48
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	8	0.48
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	7	0.48
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	7	0.48
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	14	0.48
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	11	0.48
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	13	0.47
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	13	0.47
(2,88)	1:53:A:GLN:HE22	1:56:A:GLY:HA3	2	0.47
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	8	0.47
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	8	0.47
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	12	0.47
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	12	0.47
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	12	0.47
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	12	0.47
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	12	0.47
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	12	0.47
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	6	0.47
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	6	0.47
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	17	0.47
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	13	0.47
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	13	0.47
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	13	0.47
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	19	0.47
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	19	0.47
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	19	0.47
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	4	0.47
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	4	0.47
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	4	0.47
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	13	0.47
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	13	0.47
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	13	0.47
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	10	0.47
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	2	0.47
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	2	0.47
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	2	0.47
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	2	0.47
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	8	0.47
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	8	0.47
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	8	0.47
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	8	0.47
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	3	0.47
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	3	0.47
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	13	0.47
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	17	0.47
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	7	0.47
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	7	0.47
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	7	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	3	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	3	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	3	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	4	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	4	0.47
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	4	0.47
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	14	0.47
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	14	0.47
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	14	0.47
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	14	0.47
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	14	0.47
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	14	0.47
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	6	0.47
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	6	0.47
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	19	0.47
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	19	0.47
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	12	0.47
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	12	0.47
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	3	0.47
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	3	0.47
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	18	0.47
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	18	0.47
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	12	0.47
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	18	0.47
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	8	0.47
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	11	0.47
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	3	0.47
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	3	0.47
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	3	0.47
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	2	0.47
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	2	0.47
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	19	0.47
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	19	0.47
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	18	0.47
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	14	0.47
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	17	0.47
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	8	0.47
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	15	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	15	0.47
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	2	0.47
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	2	0.47
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	12	0.47
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	12	0.47
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	12	0.47
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	1	0.47
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	1	0.47
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	1	0.47
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	8	0.47
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	8	0.47
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	8	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	14	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	14	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	14	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	14	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	14	0.47
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	14	0.47
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	17	0.47
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	4	0.47
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	13	0.47
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	7	0.47
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	20	0.47
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	18	0.47
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	9	0.47
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	9	0.47
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	9	0.47
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	13	0.47
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	10	0.47
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	5	0.47
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	12	0.47
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	14	0.47
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	15	0.47
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	15	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	3	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	3	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	9	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	9	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	11	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	11	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	14	0.47
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	4	0.47
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	8	0.47
(1,264)	1:30:A:HIS:HD1	1:31:A:HIS:H	9	0.47
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	18	0.47
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	9	0.47
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	16	0.47
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	20	0.47
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	4	0.47
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	4	0.47
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	4	0.47
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	1	0.47
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	1	0.47
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	1	0.47
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	11	0.47
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	11	0.47
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	11	0.47
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	12	0.47
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	12	0.47
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	12	0.47
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	20	0.47
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	20	0.47
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	20	0.47
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	8	0.47
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	17	0.47
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	1	0.47
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	1	0.47
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	1	0.47
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	20	0.47
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	6	0.47
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	9	0.47
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	16	0.47
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	12	0.47
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	12	0.47
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	6	0.47
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	18	0.46
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	18	0.46
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	18	0.46
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	18	0.46
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	18	0.46
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	18	0.46
(2,80)	1:11:A:TYR:HD1	1:26:A:TRP:HA	2	0.46
(2,80)	1:11:A:TYR:HD2	1:26:A:TRP:HA	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	6	0.46
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	6	0.46
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	6	0.46
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	3	0.46
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	12	0.46
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	10	0.46
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	18	0.46
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	18	0.46
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	18	0.46
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	19	0.46
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	19	0.46
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	19	0.46
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	2	0.46
(2,12)	1:16:A:ILE:H	1:55:A:GLY:HA2	14	0.46
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	2	0.46
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	18	0.46
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	14	0.46
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	14	0.46
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	19	0.46
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	1	0.46
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	1	0.46
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	1	0.46
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	1	0.46
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	1	0.46
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	1	0.46
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	1	0.46
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	3	0.46
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	3	0.46
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	13	0.46
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	13	0.46
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	15	0.46
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	15	0.46
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	8	0.46
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	8	0.46
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	12	0.46
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	12	0.46
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	5	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	5	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	5	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	16	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	16	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	16	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	20	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	20	0.46
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	20	0.46
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	1	0.46
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	1	0.46
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	1	0.46
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	1	0.46
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	1	0.46
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	1	0.46
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	11	0.46
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	11	0.46
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	8	0.46
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	8	0.46
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	11	0.46
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	11	0.46
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	2	0.46
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	2	0.46
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	2	0.46
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	2	0.46
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	14	0.46
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	14	0.46
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	14	0.46
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	14	0.46
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	1	0.46
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	1	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	5	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	9	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	10	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	15	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	16	0.46
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	18	0.46
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG2	13	0.46
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG3	13	0.46
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	10	0.46
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	20	0.46
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	15	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	15	0.46
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	15	0.46
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	4	0.46
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	8	0.46
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	3	0.46
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	14	0.46
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	20	0.46
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	5	0.46
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	5	0.46
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	5	0.46
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	4	0.46
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	4	0.46
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	7	0.46
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	7	0.46
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	1	0.46
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	6	0.46
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	12	0.46
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	12	0.46
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	4	0.46
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	13	0.46
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	13	0.46
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	13	0.46
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	11	0.46
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	2	0.46
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	14	0.46
(1,631)	1:62:A:PHE:HE1	1:72:A:ARG:H	12	0.46
(1,631)	1:62:A:PHE:HE2	1:72:A:ARG:H	12	0.46
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	11	0.46
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	11	0.46
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	11	0.46
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	20	0.46
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	20	0.46
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	20	0.46
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	5	0.46
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	11	0.46
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	5	0.46
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	13	0.46
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	7	0.46
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	10	0.46
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	15	0.46
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	17	0.46
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	11	0.46
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	11	0.46
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	1	0.46
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	1	0.46
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	1	0.46
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	11	0.46
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	18	0.46
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	18	0.46
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	18	0.46
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	4	0.46
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	8	0.46
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	17	0.46
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	18	0.46
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	18	0.46
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	19	0.46
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	9	0.46
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	3	0.46
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	12	0.46
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	2	0.46
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	2	0.46
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	5	0.46
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	5	0.46
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	5	0.46
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	13	0.46
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	13	0.46
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	13	0.46
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	16	0.46
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	16	0.46
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	16	0.46
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	19	0.46
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	19	0.46
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	19	0.46
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	4	0.46
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	10	0.46
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	5	0.46
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	5	0.46
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	5	0.46
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	14	0.46
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	14	0.46
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	14	0.46
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	11	0.46
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	18	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	19	0.46
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	19	0.46
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	19	0.46
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	1	0.45
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	1	0.45
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	1	0.45
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	1	0.45
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	1	0.45
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	1	0.45
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	1	0.45
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	10	0.45
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	9	0.45
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	9	0.45
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	13	0.45
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	14	0.45
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	8	0.45
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	8	0.45
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	8	0.45
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	12	0.45
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	12	0.45
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	12	0.45
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	10	0.45
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	10	0.45
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	10	0.45
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	1	0.45
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	7	0.45
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	17	0.45
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	17	0.45
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	11	0.45
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	11	0.45
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	15	0.45
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	15	0.45
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	15	0.45
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	6	0.45
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	6	0.45
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	6	0.45
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	6	0.45
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	6	0.45
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	6	0.45
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	6	0.45
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	6	0.45
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	6	0.45
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	6	0.45
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	6	0.45
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	2	0.45
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	2	0.45
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	8	0.45
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	8	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	3	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	3	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	3	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	6	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	6	0.45
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	6	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	2	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	2	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	2	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	15	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	15	0.45
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	15	0.45
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	7	0.45
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	7	0.45
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	3	0.45
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	3	0.45
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	10	0.45
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	10	0.45
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	16	0.45
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	16	0.45
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	20	0.45
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	20	0.45
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	7	0.45
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	7	0.45
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE1	18	0.45
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE2	18	0.45
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE1	18	0.45
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE2	18	0.45
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	19	0.45
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	19	0.45
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	19	0.45
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	12	0.45
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	12	0.45
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	6	0.45
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	1	0.45
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	17	0.45
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	17	0.45
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	5	0.45
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	5	0.45
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	16	0.45
(1,873)	1:90:A:LYS:HE2	1:91:A:ILE:H	9	0.45
(1,873)	1:90:A:LYS:HE3	1:91:A:ILE:H	9	0.45
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	17	0.45
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	14	0.45
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	19	0.45
(1,780)	1:11:A:TYR:H	1:84:A:HIS:H	5	0.45
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	7	0.45
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	13	0.45
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	13	0.45
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	20	0.45
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	5	0.45
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	12	0.45
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	12	0.45
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	4	0.45
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	16	0.45
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	16	0.45
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	20	0.45
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	9	0.45
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	1	0.45
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	2	0.45
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	4	0.45
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	18	0.45
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	17	0.45
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	19	0.45
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	10	0.45
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	14	0.45
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	17	0.45
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	9	0.45
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	9	0.45
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	9	0.45
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	20	0.45
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	20	0.45
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	17	0.45
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	10	0.45
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	5	0.45
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	5	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	16	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	16	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	16	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	17	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	17	0.45
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	17	0.45
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	2	0.45
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	2	0.45
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	2	0.45
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	14	0.45
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	3	0.45
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	7	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	7	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	7	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	7	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	10	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	10	0.45
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	10	0.45
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	6	0.45
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	16	0.45
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	16	0.45
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	6	0.45
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	6	0.45
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	20	0.45
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	20	0.45
(1,276)	1:30:A:HIS:HD1	1:32:A:LYS:H	9	0.45
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	10	0.45
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	14	0.45
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	11	0.45
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	12	0.45
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	6	0.45
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	18	0.45
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	1	0.45
(1,191)	1:25:A:THR:H	1:37:A:THR:H	16	0.45
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	13	0.45
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	13	0.45
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	5	0.45
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	17	0.45
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	11	0.45
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	6	0.45
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	6	0.45
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	1	0.45
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	16	0.45
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	1	0.45
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	7	0.45
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	7	0.45
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	7	0.45
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	4	0.45
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	3	0.45
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	3	0.45
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	3	0.45
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	11	0.44
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	11	0.44
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	11	0.44
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	4	0.44
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	8	0.44
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	11	0.44
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	7	0.44
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	7	0.44
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	7	0.44
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	7	0.44
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	7	0.44
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	7	0.44
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	20	0.44
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	16	0.44
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	19	0.44
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	1	0.44
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	1	0.44
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	1	0.44
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD21	19	0.44
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD22	19	0.44
(2,24)	1:37:A:THR:H	1:50:A:LEU:HD23	19	0.44
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	2	0.44
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	2	0.44
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	2	0.44
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	16	0.44
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	16	0.44
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	1	0.44
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	1	0.44
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	14	0.44
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	14	0.44
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	13	0.44
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	10	0.44
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	10	0.44
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	10	0.44
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	10	0.44
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	10	0.44
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	10	0.44
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	10	0.44
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	16	0.44
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	18	0.44
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	2	0.44
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	2	0.44
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	18	0.44
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	18	0.44
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	11	0.44
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	11	0.44
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	11	0.44
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	11	0.44
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	11	0.44
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	11	0.44
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	1	0.44
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	1	0.44
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	1	0.44
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	16	0.44
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	16	0.44
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	16	0.44
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	16	0.44
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	16	0.44
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	16	0.44
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	12	0.44
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	12	0.44
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	7	0.44
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	7	0.44
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	12	0.44
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	12	0.44
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	8	0.44
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	3	0.44
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	3	0.44
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	3	0.44
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	4	0.44
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	4	0.44
(1,922)	1:95:A:SER:H	1:95:A:SER:HG	14	0.44
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	13	0.44
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	9	0.44
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	9	0.44
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	7	0.44
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	18	0.44
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	6	0.44
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	6	0.44
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	6	0.44
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	17	0.44
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	14	0.44
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	14	0.44
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	19	0.44
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	19	0.44
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	20	0.44
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	20	0.44
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	13	0.44
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	1	0.44
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	2	0.44
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	4	0.44
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	4	0.44
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	5	0.44
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	13	0.44
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	13	0.44
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	13	0.44
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	6	0.44
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	6	0.44
(1,744)	1:9:A:LYS:HB2	1:81:A:GLY:H	12	0.44
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	15	0.44
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	13	0.44
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	13	0.44
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	8	0.44
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	9	0.44
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	17	0.44
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	16	0.44
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	13	0.44
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	13	0.44
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	3	0.44
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	6	0.44
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	15	0.44
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	19	0.44
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	19	0.44
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	20	0.44
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	11	0.44
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	12	0.44
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	6	0.44
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	6	0.44
(1,505)	1:53:A:GLN:H	1:61:A:ASN:HD22	16	0.44
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	14	0.44
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	14	0.44
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	14	0.44
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	9	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	18	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	18	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	18	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	20	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	20	0.44
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	20	0.44
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	5	0.44
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	9	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	10	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	10	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	10	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	12	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	12	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	12	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	15	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	15	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	15	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	18	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	18	0.44
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	18	0.44
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	17	0.44
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	18	0.44
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	7	0.44
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	10	0.44
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	11	0.44
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	4	0.44
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	4	0.44
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD1	8	0.44
(1,293)	1:33:A:VAL:H	1:34:A:TYR:HD2	8	0.44
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	20	0.44
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	18	0.44
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	14	0.44
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	15	0.44
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	10	0.44
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	9	0.44
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	10	0.44
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	17	0.44
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	16	0.44
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	8	0.44
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	8	0.44
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	19	0.44
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	19	0.44
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	2	0.44
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	2	0.44
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	2	0.44
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	3	0.44
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	3	0.44
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	3	0.44
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	9	0.44
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	9	0.44
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	9	0.44
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	17	0.44
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	17	0.44
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	17	0.44
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	2	0.44
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	11	0.44
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	9	0.44
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	1	0.44
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	2	0.43
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	2	0.43
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	2	0.43
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	2	0.43
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	2	0.43
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	2	0.43
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	3	0.43
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	7	0.43
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	2	0.43
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	5	0.43
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	16	0.43
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	16	0.43
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	16	0.43
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	19	0.43
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	19	0.43
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	19	0.43
(2,19)	1:13:A:LEU:HD11	1:29:A:LEU:H	6	0.43
(2,19)	1:13:A:LEU:HD12	1:29:A:LEU:H	6	0.43
(2,19)	1:13:A:LEU:HD13	1:29:A:LEU:H	6	0.43
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	20	0.43
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	16	0.43
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	2	0.43
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	2	0.43
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	1	0.43
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	1	0.43
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	1	0.43
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	20	0.43
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	20	0.43
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	20	0.43
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	11	0.43
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	11	0.43
(1,1103)	1:34:A:TYR:HD1	1:75:A:SER:HA	3	0.43
(1,1103)	1:34:A:TYR:HD2	1:75:A:SER:HA	3	0.43
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	11	0.43
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	20	0.43
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	20	0.43
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD1	1	0.43
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD2	1	0.43
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD1	1	0.43
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD2	1	0.43
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	20	0.43
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	20	0.43
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	20	0.43
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	20	0.43
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	4	0.43
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	4	0.43
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	7	0.43
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	7	0.43
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	6	0.43
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	6	0.43
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	6	0.43
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	6	0.43
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	6	0.43
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	9	0.43
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	9	0.43
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	9	0.43
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	9	0.43
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	9	0.43
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	9	0.43
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	1	0.43
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	1	0.43
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	17	0.43
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	17	0.43
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	17	0.43
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	2	0.43
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	2	0.43
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	2	0.43
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	2	0.43
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	2	0.43
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	2	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	1	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	1	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	3	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	3	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	5	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	5	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	6	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	6	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	8	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	8	0.43
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	9	0.43
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	9	0.43
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	6	0.43
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	6	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	1	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	1	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	3	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	3	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	5	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	5	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	6	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	8	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	8	0.43
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	9	0.43
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	9	0.43
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	20	0.43
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	20	0.43
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	8	0.43
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	8	0.43
(1,947)	1:95:A:SER:HA	1:98:A:LEU:H	4	0.43
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	6	0.43
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	6	0.43
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	8	0.43
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	11	0.43
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	11	0.43
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	16	0.43
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	4	0.43
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	4	0.43
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	7	0.43
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	7	0.43
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	12	0.43
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	12	0.43
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	17	0.43
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	17	0.43
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	3	0.43
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	7	0.43
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	9	0.43
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	11	0.43
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	7	0.43
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	9	0.43
(1,764)	1:13:A:LEU:HD11	1:83:A:LEU:H	12	0.43
(1,764)	1:13:A:LEU:HD12	1:83:A:LEU:H	12	0.43
(1,764)	1:13:A:LEU:HD13	1:83:A:LEU:H	12	0.43
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	16	0.43
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	16	0.43
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	16	0.43
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	10	0.43
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	10	0.43
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	19	0.43
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	19	0.43
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	11	0.43
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	13	0.43
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	14	0.43
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	10	0.43
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	3	0.43
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	7	0.43
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	13	0.43
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	16	0.43
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	9	0.43
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	16	0.43
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	1	0.43
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	8	0.43
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	11	0.43
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	11	0.43
(1,505)	1:53:A:GLN:H	1:61:A:ASN:HD22	10	0.43
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	3	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	7	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	7	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	7	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	8	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	8	0.43
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	8	0.43
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	6	0.43
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	6	0.43
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	2	0.43
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	2	0.43
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	2	0.43
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	18	0.43
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	18	0.43
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	18	0.43
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	7	0.43
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	7	0.43
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	4	0.43
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	7	0.43
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	7	0.43
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	7	0.43
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	7	0.43
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	19	0.43
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	11	0.43
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	11	0.43
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	7	0.43
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	17	0.43
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	18	0.43
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	2	0.43
(1,191)	1:25:A:THR:H	1:37:A:THR:H	1	0.43
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	5	0.43
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	5	0.43
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	7	0.43
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	8	0.43
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	8	0.43
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	8	0.43
(1,101)	1:12:A:THR:HG21	1:15:A:GLU:H	15	0.43
(1,101)	1:12:A:THR:HG22	1:15:A:GLU:H	15	0.43
(1,101)	1:12:A:THR:HG23	1:15:A:GLU:H	15	0.43
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	2	0.43
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	18	0.43
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	5	0.43
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	20	0.43
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	0.43
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	11	0.43
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB2	20	0.42
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB3	20	0.42
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	6	0.42
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	6	0.42
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	6	0.42
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	6	0.42
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	6	0.42
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	6	0.42
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	13	0.42
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	4	0.42
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	4	0.42
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	4	0.42
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	4	0.42
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	4	0.42
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	4	0.42
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	5	0.42
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	18	0.42
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	13	0.42
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	4	0.42
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	1	0.42
(1,1083)	1:53:A:GLN:HE22	1:64:A:ASP:HB2	4	0.42
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	12	0.42
(1,1060)	1:39:A:PHE:HD1	1:75:A:SER:HA	4	0.42
(1,1060)	1:39:A:PHE:HD2	1:75:A:SER:HA	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	9	0.42
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	9	0.42
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	14	0.42
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	14	0.42
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	14	0.42
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	14	0.42
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	14	0.42
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	14	0.42
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	14	0.42
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	18	0.42
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	18	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	3	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	3	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	3	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	3	0.42
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	3	0.42
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	3	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	4	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	4	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	4	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	4	0.42
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	4	0.42
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	4	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	10	0.42
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	10	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	10	0.42
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	10	0.42
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	10	0.42
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	18	0.42
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	18	0.42
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	12	0.42
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	12	0.42
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	14	0.42
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	14	0.42
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	7	0.42
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	7	0.42
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	9	0.42
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	9	0.42
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	9	0.42
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	9	0.42
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	9	0.42
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	9	0.42
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	17	0.42
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	17	0.42
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	5	0.42
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	5	0.42
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	11	0.42
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	11	0.42
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	15	0.42
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	15	0.42
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	17	0.42
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	17	0.42
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	17	0.42
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	17	0.42
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	15	0.42
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	15	0.42
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	15	0.42
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	15	0.42
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	19	0.42
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	19	0.42
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	19	0.42
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	19	0.42
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA2	10	0.42
(1,955)	1:32:A:LYS:HD3	1:81:A:GLY:HA3	10	0.42
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	7	0.42
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	7	0.42
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	7	0.42
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	5	0.42
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	16	0.42
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	5	0.42
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	5	0.42
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	5	0.42
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	11	0.42
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	11	0.42
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	11	0.42
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	12	0.42
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	12	0.42
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	12	0.42
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	17	0.42
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	17	0.42
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	17	0.42
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	13	0.42
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	20	0.42
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	16	0.42
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	16	0.42
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	8	0.42
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	19	0.42
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	15	0.42
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	5	0.42
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	13	0.42
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	12	0.42
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	12	0.42
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	12	0.42
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	14	0.42
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	14	0.42
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	15	0.42
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	15	0.42
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	20	0.42
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	20	0.42
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	2	0.42
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	10	0.42
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	10	0.42
(1,659)	1:75:A:SER:H	1:78:A:TYR:HB2	3	0.42
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	13	0.42
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	13	0.42
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	13	0.42
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	16	0.42
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	17	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	13	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	13	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	13	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	13	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	13	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	16	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	16	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	16	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	16	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	16	0.42
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	16	0.42
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	11	0.42
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	14	0.42
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	18	0.42
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	9	0.42
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	17	0.42
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	18	0.42
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	1	0.42
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	10	0.42
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	20	0.42
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	12	0.42
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	16	0.42
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	2	0.42
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	15	0.42
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	9	0.42
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	9	0.42
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	14	0.42
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	14	0.42
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	8	0.42
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	15	0.42
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	15	0.42
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	5	0.42
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	3	0.42
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	3	0.42
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	3	0.42
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	12	0.42
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	11	0.42
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	15	0.42
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	15	0.42
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	15	0.42
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	9	0.42
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	13	0.42
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	6	0.42
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	15	0.42
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	15	0.42
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	15	0.42
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	4	0.42
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	15	0.42
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	5	0.42
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	9	0.42
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	13	0.42
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	19	0.42
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	5	0.42
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	12	0.42
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	2	0.42
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	2	0.42
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	2	0.42
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	13	0.42
(1,191)	1:25:A:THR:H	1:37:A:THR:H	7	0.42
(1,191)	1:25:A:THR:H	1:37:A:THR:H	18	0.42
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	10	0.42
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	4	0.42
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	16	0.42
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	3	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	2	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	2	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	2	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	5	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	5	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	5	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	14	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	14	0.42
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	14	0.42
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	10	0.42
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	13	0.41
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	15	0.41
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	9	0.41
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	9	0.41
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	10	0.41
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	10	0.41
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	10	0.41
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	20	0.41
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	20	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	20	0.41
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	14	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	5	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	5	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	15	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	15	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	18	0.41
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	18	0.41
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	3	0.41
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	9	0.41
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	15	0.41
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	15	0.41
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	9	0.41
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	9	0.41
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	6	0.41
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	6	0.41
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	9	0.41
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	13	0.41
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	13	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	5	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	5	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	5	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	5	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	5	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	5	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	7	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	7	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	7	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	7	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	7	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	7	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	8	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	8	0.41
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	8	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	8	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	8	0.41
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	8	0.41
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	10	0.41
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	10	0.41
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	10	0.41
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	5	0.41
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	5	0.41
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	5	0.41
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	5	0.41
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	5	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	4	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	4	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	4	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	4	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	4	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	4	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	6	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	6	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	6	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	6	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	6	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	6	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	9	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	9	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	9	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	9	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	9	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	9	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	15	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	15	0.41
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	15	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	15	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	15	0.41
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	15	0.41
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	4	0.41
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	4	0.41
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	4	0.41
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	4	0.41
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	12	0.41
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	11	0.41
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	11	0.41
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	1	0.41
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	10	0.41
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	12	0.41
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	2	0.41
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	12	0.41
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	5	0.41
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	18	0.41
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	2	0.41
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	1	0.41
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	1	0.41
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	1	0.41
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	14	0.41
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	11	0.41
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	11	0.41
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	20	0.41
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	6	0.41
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	12	0.41
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	18	0.41
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	7	0.41
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	10	0.41
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	2	0.41
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	2	0.41
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	2	0.41
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	3	0.41
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	3	0.41
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	4	0.41
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	12	0.41
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	12	0.41
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	12	0.41
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	18	0.41
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	8	0.41
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	8	0.41
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	3	0.41
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	3	0.41
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	7	0.41
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	17	0.41
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	1	0.41
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	3	0.41
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	9	0.41
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	12	0.41
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	12	0.41
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	12	0.41
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	18	0.41
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	18	0.41
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	18	0.41
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	14	0.41
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	7	0.41
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:58:A:ALA:H	1:61:A:ASN:H	9	0.41
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	1	0.41
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	13	0.41
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	3	0.41
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	9	0.41
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	19	0.41
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	17	0.41
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	5	0.41
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	17	0.41
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	20	0.41
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	20	0.41
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	10	0.41
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	10	0.41
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	10	0.41
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	3	0.41
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	1	0.41
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	1	0.41
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	1	0.41
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	18	0.41
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	18	0.41
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	20	0.41
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	5	0.41
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	5	0.41
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	8	0.41
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	8	0.41
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	15	0.41
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	15	0.41
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	3	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	7	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	7	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	7	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	10	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	10	0.41
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	10	0.41
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	1	0.41
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	4	0.41
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	8	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	1	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	1	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	1	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	6	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	6	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	8	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	8	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	8	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	13	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	13	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	13	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	16	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	16	0.41
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	16	0.41
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	14	0.41
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	3	0.41
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	3	0.41
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	3	0.41
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	6	0.41
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	19	0.41
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	2	0.41
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	2	0.41
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	5	0.41
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	5	0.41
(1,263)	1:30:A:HIS:HE1	1:31:A:HIS:H	16	0.41
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	5	0.41
(1,233)	1:13:A:LEU:HD11	1:28:A:ILE:H	12	0.41
(1,233)	1:13:A:LEU:HD12	1:28:A:ILE:H	12	0.41
(1,233)	1:13:A:LEU:HD13	1:28:A:ILE:H	12	0.41
(1,233)	1:13:A:LEU:HD21	1:28:A:ILE:H	12	0.41
(1,233)	1:13:A:LEU:HD22	1:28:A:ILE:H	12	0.41
(1,233)	1:13:A:LEU:HD23	1:28:A:ILE:H	12	0.41
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	4	0.41
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	6	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	7	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	7	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	7	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	18	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	18	0.41
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	18	0.41
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	13	0.41
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	14	0.41
(1,191)	1:25:A:THR:H	1:37:A:THR:H	10	0.41
(1,191)	1:25:A:THR:H	1:37:A:THR:H	20	0.41
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	4	0.41
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	18	0.41
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	11	0.41
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	9	0.41
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	9	0.41
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	14	0.41
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	14	0.41
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	11	0.41
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	11	0.41
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	11	0.41
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	19	0.41
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	19	0.41
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	3	0.41
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	15	0.41
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	6	0.41
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	15	0.41
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	15	0.41
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	15	0.41
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	12	0.41
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	4	0.41
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	11	0.41
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	18	0.41
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	5	0.41
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	5	0.41
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	7	0.41
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	11	0.4
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	11	0.4
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	10	0.4
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	10	0.4
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	10	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	10	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	10	0.4
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	10	0.4
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	10	0.4
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	20	0.4
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	16	0.4
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	7	0.4
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	2	0.4
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	2	0.4
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	2	0.4
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	5	0.4
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	5	0.4
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	11	0.4
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	11	0.4
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	11	0.4
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	10	0.4
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	10	0.4
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	10	0.4
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	10	0.4
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	20	0.4
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	20	0.4
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	20	0.4
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	20	0.4
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	7	0.4
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	7	0.4
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	7	0.4
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	7	0.4
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	7	0.4
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	7	0.4
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	7	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	1	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	1	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	1	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	1	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	1	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	1	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	2	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	2	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	2	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	2	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	2	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	2	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	11	0.4
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	11	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	11	0.4
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	11	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	11	0.4
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	11	0.4
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	4	0.4
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	5	0.4
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	5	0.4
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	1	0.4
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	1	0.4
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	8	0.4
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	8	0.4
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	3	0.4
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	3	0.4
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	20	0.4
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	20	0.4
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	11	0.4
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	11	0.4
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	11	0.4
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	7	0.4
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	7	0.4
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	7	0.4
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	7	0.4
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	7	0.4
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	7	0.4
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	20	0.4
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	20	0.4
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	20	0.4
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	20	0.4
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	20	0.4
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	20	0.4
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	18	0.4
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	18	0.4
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	17	0.4
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	17	0.4
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	1	0.4
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	6	0.4
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	14	0.4
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	16	0.4
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	16	0.4
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	16	0.4
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	16	0.4
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	5	0.4
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	4	0.4
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	17	0.4
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	20	0.4
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:86:A:ASP:H	1:87:A:ASP:HB2	16	0.4
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	6	0.4
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	8	0.4
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	14	0.4
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	14	0.4
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	14	0.4
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	1	0.4
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	1	0.4
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	9	0.4
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	9	0.4
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	11	0.4
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	11	0.4
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	1	0.4
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	8	0.4
(1,744)	1:9:A:LYS:HB2	1:81:A:GLY:H	5	0.4
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	7	0.4
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	7	0.4
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	7	0.4
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	8	0.4
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	8	0.4
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	14	0.4
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	14	0.4
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	20	0.4
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	20	0.4
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	19	0.4
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	20	0.4
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	5	0.4
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	5	0.4
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	13	0.4
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	12	0.4
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	12	0.4
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	15	0.4
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	20	0.4
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	19	0.4
(1,622)	1:70:A:ASP:HB2	1:71:A:ALA:H	13	0.4
(1,622)	1:70:A:ASP:HB3	1:71:A:ALA:H	13	0.4
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	17	0.4
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	17	0.4
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	17	0.4
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	7	0.4
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	3	0.4
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	10	0.4
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	5	0.4
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	8	0.4
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	1	0.4
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	5	0.4
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	10	0.4
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	19	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	3	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	3	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	3	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	11	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	11	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	11	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	15	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	15	0.4
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	15	0.4
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	7	0.4
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	17	0.4
(1,431)	1:39:A:PHE:HA	1:43:A:TRP:H	7	0.4
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	20	0.4
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	20	0.4
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	2	0.4
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	13	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	16	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	16	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	16	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	17	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	17	0.4
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	17	0.4
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	5	0.4
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	12	0.4
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	12	0.4
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	6	0.4
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	13	0.4
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	3	0.4
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	4	0.4
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	10	0.4
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	16	0.4
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	17	0.4
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	6	0.4
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	19	0.4
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	19	0.4
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	20	0.4
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	14	0.4
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	14	0.4
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	14	0.4
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	6	0.4
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	6	0.4
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	11	0.4
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	11	0.4
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	11	0.4
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	12	0.4
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	16	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	1	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	1	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	1	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	9	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	9	0.4
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	9	0.4
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	12	0.4
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	2	0.4
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	4	0.4
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	4	0.4
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	16	0.4
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	6	0.4
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	3	0.4
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	3	0.4
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	3	0.4
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	16	0.4
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	3	0.4
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	17	0.4
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	17	0.4
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	20	0.4
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	18	0.39
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	18	0.39
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	18	0.39
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	10	0.39
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	10	0.39
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	10	0.39
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	5	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	3	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	3	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	3	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	3	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	3	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	11	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	11	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	11	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	11	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	11	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	11	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	19	0.39
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	19	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	19	0.39
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	19	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	19	0.39
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	19	0.39
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	19	0.39
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	10	0.39
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	5	0.39
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	5	0.39
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	5	0.39
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	5	0.39
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	11	0.39
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	8	0.39
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	13	0.39
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	13	0.39
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	6	0.39
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	6	0.39
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	6	0.39
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	9	0.39
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	9	0.39
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	9	0.39
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	15	0.39
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	15	0.39
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	15	0.39
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	15	0.39
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	19	0.39
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	10	0.39
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	10	0.39
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	2	0.39
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	2	0.39
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	2	0.39
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	9	0.39
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	13	0.39
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	13	0.39
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	4	0.39
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	4	0.39
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	6	0.39
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	6	0.39
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	9	0.39
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	9	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	14	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	14	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	14	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	14	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	14	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	14	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	20	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	20	0.39
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	20	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	20	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	20	0.39
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	20	0.39
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	11	0.39
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	11	0.39
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	11	0.39
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	11	0.39
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	11	0.39
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	11	0.39
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	8	0.39
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	8	0.39
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	8	0.39
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	8	0.39
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	8	0.39
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	8	0.39
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	2	0.39
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	2	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	10	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	10	0.39
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	10	0.39
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	10	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	16	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	16	0.39
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	16	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	17	0.39
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	17	0.39
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	17	0.39
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	17	0.39
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD1	18	0.39
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD2	18	0.39
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	3	0.39
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	3	0.39
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	4	0.39
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	7	0.39
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	12	0.39
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	1	0.39
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	12	0.39
(1,873)	1:90:A:LYS:HE2	1:91:A:ILE:H	1	0.39
(1,873)	1:90:A:LYS:HE3	1:91:A:ILE:H	1	0.39
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	8	0.39
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	8	0.39
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	8	0.39
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	1	0.39
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	8	0.39
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	6	0.39
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	9	0.39
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	5	0.39
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	20	0.39
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	14	0.39
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	7	0.39
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	7	0.39
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	7	0.39
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	19	0.39
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	10	0.39
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	10	0.39
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	10	0.39
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	3	0.39
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	3	0.39
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	5	0.39
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	11	0.39
(1,689)	1:74:A:LEU:HA	1:78:A:TYR:H	13	0.39
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	8	0.39
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	13	0.39
(1,662)	1:62:A:PHE:HD1	1:76:A:LYS:H	16	0.39
(1,662)	1:62:A:PHE:HD2	1:76:A:LYS:H	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	14	0.39
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	13	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	5	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	5	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	5	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	5	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	5	0.39
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	5	0.39
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	20	0.39
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	20	0.39
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	7	0.39
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	2	0.39
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	2	0.39
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	4	0.39
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	18	0.39
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	3	0.39
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	11	0.39
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	14	0.39
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	16	0.39
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	6	0.39
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	13	0.39
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	13	0.39
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	13	0.39
(1,457)	1:46:A:GLY:H	1:49:A:VAL:H	18	0.39
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	12	0.39
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	6	0.39
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	6	0.39
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	16	0.39
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	16	0.39
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	14	0.39
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	4	0.39
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	9	0.39
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	8	0.39
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	8	0.39
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	8	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	7	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	7	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	7	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	11	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	11	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	11	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	14	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	14	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	20	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	20	0.39
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	20	0.39
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	5	0.39
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	5	0.39
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	5	0.39
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	11	0.39
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	16	0.39
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	2	0.39
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	2	0.39
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	2	0.39
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	8	0.39
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	6	0.39
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	6	0.39
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	9	0.39
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	9	0.39
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	19	0.39
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	19	0.39
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	7	0.39
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	16	0.39
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	14	0.39
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	16	0.39
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	10	0.39
(1,241)	1:29:A:LEU:H	1:83:A:LEU:HG	2	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	8	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	8	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	8	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	9	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	9	0.39
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	9	0.39
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	3	0.39
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	16	0.39
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	7	0.39
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	7	0.39
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	7	0.39
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	7	0.39
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	20	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	8	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	8	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	15	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	16	0.39
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	16	0.39
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	9	0.39
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	9	0.39
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	13	0.39
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	20	0.39
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	8	0.39
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	8	0.39
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	8	0.39
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	5	0.39
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	16	0.39
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	14	0.38
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	15	0.38
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	20	0.38
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	17	0.38
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	3	0.38
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	3	0.38
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	4	0.38
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	4	0.38
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	4	0.38
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	17	0.38
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	2	0.38
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	13	0.38
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	13	0.38
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	6	0.38
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	10	0.38
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	10	0.38
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	10	0.38
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	10	0.38
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	12	0.38
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	12	0.38
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	12	0.38
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	12	0.38
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	12	0.38
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	12	0.38
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	20	0.38
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	20	0.38
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	20	0.38
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	20	0.38
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	20	0.38
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	20	0.38
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	20	0.38
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	1	0.38
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	1	0.38
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	7	0.38
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	7	0.38
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	5	0.38
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	5	0.38
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	12	0.38
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	12	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	7	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	7	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	7	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	7	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	7	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	7	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	14	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	14	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	14	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	14	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	14	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	14	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	20	0.38
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	20	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	20	0.38
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	20	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	20	0.38
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	20	0.38
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	5	0.38
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	5	0.38
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	18	0.38
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	9	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	9	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	9	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	9	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	9	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	9	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	15	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	15	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	15	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	15	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	15	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	15	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	16	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	16	0.38
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	16	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	16	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	16	0.38
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	16	0.38
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG21	9	0.38
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG22	9	0.38
(1,994)	1:11:A:TYR:HA	1:33:A:VAL:HG23	9	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	1	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	1	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	1	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	1	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	1	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	1	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	3	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	3	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	3	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	3	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	3	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	3	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	10	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	10	0.38
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	10	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	10	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	10	0.38
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	10	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	14	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	14	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	14	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	14	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	14	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	17	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	17	0.38
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	17	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	17	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	17	0.38
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	17	0.38
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	2	0.38
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	2	0.38
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	5	0.38
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	18	0.38
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	16	0.38
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	7	0.38
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	5	0.38
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	2	0.38
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	14	0.38
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	14	0.38
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	14	0.38
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	15	0.38
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	9	0.38
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	2	0.38
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	2	0.38
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	8	0.38
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	5	0.38
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	5	0.38
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	6	0.38
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	4	0.38
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	4	0.38
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	4	0.38
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	16	0.38
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	16	0.38
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	19	0.38
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	19	0.38
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	16	0.38
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	19	0.38
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	2	0.38
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	18	0.38
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	5	0.38
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	7	0.38
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	8	0.38
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	19	0.38
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	16	0.38
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	19	0.38
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	19	0.38
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	6	0.38
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	16	0.38
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	6	0.38
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	15	0.38
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	19	0.38
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	10	0.38
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	10	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	1	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	2	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	4	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	10	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	13	0.38
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	18	0.38
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	20	0.38
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	2	0.38
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	13	0.38
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	13	0.38
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	13	0.38
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	14	0.38
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	5	0.38
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	5	0.38
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	5	0.38
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	10	0.38
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	10	0.38
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	3	0.38
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	13	0.38
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	13	0.38
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	6	0.38
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	6	0.38
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	6	0.38
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	3	0.38
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	18	0.38
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	2	0.38
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	2	0.38
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	2	0.38
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	17	0.38
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	17	0.38
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	13	0.38
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	13	0.38
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	13	0.38
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	3	0.38
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	3	0.38
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	3	0.38
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	3	0.38
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	3	0.38
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	9	0.38
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	19	0.38
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	4	0.38
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	16	0.38
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	16	0.38
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	16	0.38
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	6	0.38
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	10	0.38
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	9	0.38
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	20	0.38
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	1	0.38
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	1	0.38
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	4	0.38
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	4	0.38
(1,275)	1:32:A:LYS:H	1:83:A:LEU:HG	13	0.38
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	16	0.38
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	18	0.38
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	7	0.38
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	2	0.38
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	2	0.38
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	2	0.38
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	17	0.38
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	1	0.38
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	1	0.38
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	1	0.38
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	10	0.38
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	10	0.38
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	10	0.38
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	18	0.38
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	18	0.38
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	18	0.38
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	20	0.38
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	20	0.38
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	13	0.38
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	17	0.38
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	10	0.38
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	18	0.38
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	18	0.38
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	18	0.38
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	14	0.38
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	6	0.38
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	6	0.38
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	18	0.38
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	18	0.38
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	19	0.37
(2,84)	1:39:A:PHE:HE1	1:42:A:GLU:HB3	1	0.37
(2,84)	1:39:A:PHE:HE2	1:42:A:GLU:HB3	1	0.37
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	14	0.37
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	14	0.37
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	14	0.37
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	11	0.37
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	11	0.37
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	16	0.37
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	16	0.37
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	20	0.37
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	20	0.37
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	20	0.37
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	12	0.37
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	3	0.37
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	3	0.37
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	10	0.37
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	12	0.37
(2,2)	1:10:A:TYR:H	1:84:A:HIS:HD2	4	0.37
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	1	0.37
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	1	0.37
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	11	0.37
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	11	0.37
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	9	0.37
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	9	0.37
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	9	0.37
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	9	0.37
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	9	0.37
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	9	0.37
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	18	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	18	0.37
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	18	0.37
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	18	0.37
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	18	0.37
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	18	0.37
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	18	0.37
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	18	0.37
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	18	0.37
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	18	0.37
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	18	0.37
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	18	0.37
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	14	0.37
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	14	0.37
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	1	0.37
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	1	0.37
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	1	0.37
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	1	0.37
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	6	0.37
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	6	0.37
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	4	0.37
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	4	0.37
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	10	0.37
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	10	0.37
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	15	0.37
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	15	0.37
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	19	0.37
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	19	0.37
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	12	0.37
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	12	0.37
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	8	0.37
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	8	0.37
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	8	0.37
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	17	0.37
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	17	0.37
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	17	0.37
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	17	0.37
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	17	0.37
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	17	0.37
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	19	0.37
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	19	0.37
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	19	0.37
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	19	0.37
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	19	0.37
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	16	0.37
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	16	0.37
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	18	0.37
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	18	0.37
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	16	0.37
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	16	0.37
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	18	0.37
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	18	0.37
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	6	0.37
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	12	0.37
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	20	0.37
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	5	0.37
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	7	0.37
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	7	0.37
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	4	0.37
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	16	0.37
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	17	0.37
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	4	0.37
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	18	0.37
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	10	0.37
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	10	0.37
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	14	0.37
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	20	0.37
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	4	0.37
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	9	0.37
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	13	0.37
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	17	0.37
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	7	0.37
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	17	0.37
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	6	0.37
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	6	0.37
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	6	0.37
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	10	0.37
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	10	0.37
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	2	0.37
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	2	0.37
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	2	0.37
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	5	0.37
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	5	0.37
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	14	0.37
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	14	0.37
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	14	0.37
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	9	0.37
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	19	0.37
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	15	0.37
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	3	0.37
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	3	0.37
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	2	0.37
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	2	0.37
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	7	0.37
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	7	0.37
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	15	0.37
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	15	0.37
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	16	0.37
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	8	0.37
(1,631)	1:62:A:PHE:HE1	1:72:A:ARG:H	5	0.37
(1,631)	1:62:A:PHE:HE2	1:72:A:ARG:H	5	0.37
(1,630)	1:39:A:PHE:HZ	1:72:A:ARG:H	9	0.37
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	19	0.37
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	19	0.37
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	19	0.37
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	7	0.37
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	7	0.37
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	7	0.37
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	10	0.37
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	4	0.37
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	3	0.37
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	13	0.37
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	3	0.37
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	7	0.37
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	13	0.37
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	16	0.37
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	16	0.37
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	16	0.37
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	17	0.37
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	6	0.37
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	9	0.37
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	14	0.37
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	3	0.37
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	3	0.37
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	14	0.37
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	14	0.37
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	14	0.37
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	15	0.37
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	3	0.37
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	3	0.37
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	3	0.37
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	13	0.37
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	7	0.37
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	10	0.37
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	11	0.37
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	20	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	6	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	6	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	6	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	13	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	13	0.37
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	13	0.37
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	9	0.37
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	13	0.37
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	11	0.37
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	3	0.37
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	6	0.37
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	6	0.37
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	19	0.37
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	16	0.37
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	9	0.37
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	17	0.37
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	6	0.37
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	15	0.37
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	15	0.37
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	15	0.37
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	2	0.37
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	6	0.37
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	6	0.37
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	6	0.37
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	8	0.37
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	4	0.37
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	13	0.37
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	13	0.37
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	13	0.37
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	4	0.37
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	11	0.37
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	4	0.37
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	20	0.37
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	20	0.37
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	1	0.37
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	1	0.37
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	1	0.37
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	3	0.37
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	6	0.37
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	6	0.37
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	9	0.37
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	15	0.36
(3,24)	1:37:A:THR:O	1:41:A:GLU:H	12	0.36
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	13	0.36
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	3	0.36
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	3	0.36
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	3	0.36
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	3	0.36
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	3	0.36
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	3	0.36
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	6	0.36
(2,76)	1:25:A:THR:HA	1:26:A:TRP:HD1	12	0.36
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	16	0.36
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	5	0.36
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	12	0.36
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	9	0.36
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	6	0.36
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	18	0.36
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	9	0.36
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	4	0.36
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	4	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	8	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	8	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	12	0.36
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	12	0.36
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	17	0.36
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	17	0.36
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	17	0.36
(1,1081)	1:53:A:GLN:HE22	1:64:A:ASP:HB3	12	0.36
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	2	0.36
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	2	0.36
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	2	0.36
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	2	0.36
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	2	0.36
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	2	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	11	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	11	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	15	0.36
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	15	0.36
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	5	0.36
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	3	0.36
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	3	0.36
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	14	0.36
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	14	0.36
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	16	0.36
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	16	0.36
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	17	0.36
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	17	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	4	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	4	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	4	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	4	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	4	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	4	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	13	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	13	0.36
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	13	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	13	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	13	0.36
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	13	0.36
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	8	0.36
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	8	0.36
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	8	0.36
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	8	0.36
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	8	0.36
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	8	0.36
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	3	0.36
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	3	0.36
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	3	0.36
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	3	0.36
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	3	0.36
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	6	0.36
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	6	0.36
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	4	0.36
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	4	0.36
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	4	0.36
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	4	0.36
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	6	0.36
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	6	0.36
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	6	0.36
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	6	0.36
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	14	0.36
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	14	0.36
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	19	0.36
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG2	14	0.36
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG3	14	0.36
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	1	0.36
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	8	0.36
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	1	0.36
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	3	0.36
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	11	0.36
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	15	0.36
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	14	0.36
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	1	0.36
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	1	0.36
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	12	0.36
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	6	0.36
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	6	0.36
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	8	0.36
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	15	0.36
(1,778)	1:84:A:HIS:H	1:84:A:HIS:HD2	4	0.36
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	2	0.36
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	15	0.36
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	4	0.36
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	15	0.36
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	10	0.36
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	10	0.36
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	18	0.36
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	18	0.36
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	18	0.36
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	8	0.36
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	8	0.36
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	20	0.36
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	4	0.36
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	18	0.36
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	18	0.36
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	6	0.36
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	7	0.36
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	7	0.36
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	14	0.36
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	6	0.36
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	20	0.36
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	8	0.36
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	8	0.36
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	3	0.36
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	9	0.36
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	17	0.36
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	18	0.36
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	20	0.36
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	11	0.36
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	9	0.36
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	6	0.36
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	15	0.36
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	12	0.36
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	3	0.36
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	15	0.36
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	2	0.36
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	18	0.36
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	7	0.36
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	12	0.36
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	15	0.36
(1,507)	1:53:A:GLN:HA	1:54:A:ALA:H	19	0.36
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	8	0.36
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	15	0.36
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	15	0.36
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	15	0.36
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	17	0.36
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	17	0.36
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	2	0.36
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	14	0.36
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	14	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	12	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	12	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	12	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	13	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	13	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	13	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	14	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	14	0.36
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	14	0.36
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	8	0.36
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	3	0.36
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	10	0.36
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	16	0.36
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	18	0.36
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	12	0.36
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	2	0.36
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	17	0.36
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	17	0.36
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	17	0.36
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	17	0.36
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	10	0.36
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	20	0.36
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	20	0.36
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	6	0.36
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	8	0.36
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	11	0.36
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	1	0.36
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	10	0.36
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	18	0.36
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	11	0.36
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	18	0.36
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	13	0.36
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	16	0.36
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	16	0.36
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	16	0.36
(1,191)	1:25:A:THR:H	1:37:A:THR:H	2	0.36
(1,171)	1:23:A:LYS:H	1:25:A:THR:HG1	9	0.36
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	13	0.36
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	13	0.36
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	6	0.36
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	13	0.36
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	8	0.36
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	11	0.36
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	17	0.36
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	7	0.36
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	2	0.36
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	2	0.36
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	8	0.36
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	8	0.36
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	15	0.36
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	15	0.36
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	15	0.36
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	7	0.35
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	7	0.35
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	7	0.35
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	7	0.35
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	3	0.35
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	15	0.35
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	7	0.35
(2,31)	1:50:A:LEU:HD21	1:52:A:GLU:H	7	0.35
(2,31)	1:50:A:LEU:HD22	1:52:A:GLU:H	7	0.35
(2,31)	1:50:A:LEU:HD23	1:52:A:GLU:H	7	0.35
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	13	0.35
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	13	0.35
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	13	0.35
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG21	3	0.35
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG22	3	0.35
(2,27)	1:46:A:GLY:H	1:49:A:VAL:HG23	3	0.35
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	12	0.35
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	12	0.35
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	6	0.35
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	6	0.35
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	3	0.35
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	3	0.35
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	3	0.35
(1,1088)	1:61:A:ASN:HD21	1:62:A:PHE:HA	7	0.35
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	19	0.35
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	15	0.35
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	15	0.35
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	15	0.35
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	15	0.35
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	15	0.35
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	15	0.35
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	19	0.35
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	19	0.35
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	19	0.35
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	19	0.35
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	19	0.35
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	19	0.35
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	19	0.35
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	7	0.35
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	7	0.35
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	15	0.35
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	15	0.35
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	15	0.35
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	15	0.35
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	15	0.35
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	15	0.35
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	2	0.35
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	2	0.35
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	10	0.35
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	10	0.35
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	7	0.35
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	20	0.35
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	20	0.35
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	18	0.35
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	18	0.35
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	18	0.35
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	18	0.35
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	18	0.35
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	18	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	10	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	10	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	10	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	11	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	11	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	11	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	14	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	14	0.35
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	14	0.35
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	18	0.35
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	18	0.35
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	18	0.35
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	18	0.35
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	18	0.35
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	18	0.35
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	7	0.35
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	7	0.35
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	7	0.35
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	7	0.35
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	7	0.35
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	7	0.35
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	15	0.35
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	15	0.35
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	15	0.35
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	15	0.35
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	1	0.35
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	1	0.35
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	11	0.35
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	11	0.35
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	14	0.35
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	14	0.35
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	3	0.35
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	3	0.35
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	3	0.35
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	3	0.35
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG11	15	0.35
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG12	15	0.35
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG13	15	0.35
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG2	18	0.35
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG3	18	0.35
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	15	0.35
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	20	0.35
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	9	0.35
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	9	0.35
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	9	0.35
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	5	0.35
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	19	0.35
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	4	0.35
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	4	0.35
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	4	0.35
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	18	0.35
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	20	0.35
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	10	0.35
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	7	0.35
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	3	0.35
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	4	0.35
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	10	0.35
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	16	0.35
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	19	0.35
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	19	0.35
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	3	0.35
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	7	0.35
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	7	0.35
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	11	0.35
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	11	0.35
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	11	0.35
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	16	0.35
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	12	0.35
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	12	0.35
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	15	0.35
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	15	0.35
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	9	0.35
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	14	0.35
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	14	0.35
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	11	0.35
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	11	0.35
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	10	0.35
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	10	0.35
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	12	0.35
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	13	0.35
(1,647)	1:62:A:PHE:HB2	1:75:A:SER:H	2	0.35
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	19	0.35
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	15	0.35
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	15	0.35
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	16	0.35
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	16	0.35
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	16	0.35
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	14	0.35
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	11	0.35
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	11	0.35
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	11	0.35
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	13	0.35
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	13	0.35
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	13	0.35
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	16	0.35
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	2	0.35
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	20	0.35
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	20	0.35
(1,532)	1:58:A:ALA:H	1:61:A:ASN:H	9	0.35
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	2	0.35
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	2	0.35
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	2	0.35
(1,482)	1:40:A:LEU:HB3	1:51:A:ARG:H	13	0.35
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	7	0.35
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	8	0.35
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	12	0.35
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	20	0.35
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	9	0.35
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	6	0.35
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	13	0.35
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	19	0.35
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	15	0.35
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	2	0.35
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	1	0.35
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	18	0.35
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	1	0.35
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	1	0.35
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	19	0.35
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	19	0.35
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	2	0.35
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	2	0.35
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	3	0.35
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	3	0.35
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	12	0.35
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	14	0.35
(1,263)	1:30:A:HIS:HE1	1:31:A:HIS:H	18	0.35
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	13	0.35
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	20	0.35
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	7	0.35
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	7	0.35
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	7	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	17	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	17	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	17	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	20	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	20	0.35
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	20	0.35
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	12	0.35
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	20	0.35
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	12	0.35
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	12	0.35
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	12	0.35
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	16	0.35
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	16	0.35
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	16	0.35
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	17	0.35
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	17	0.35
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	17	0.35
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	20	0.35
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	20	0.35
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	20	0.35
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	13	0.35
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	14	0.35
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	15	0.35
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	4	0.35
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	4	0.35
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	5	0.35
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	5	0.35
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	5	0.35
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	5	0.35
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	17	0.35
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	17	0.35
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	17	0.35
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	7	0.35
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	13	0.35
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	3	0.35
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	3	0.35
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	4	0.35
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	4	0.35
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	14	0.35
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	14	0.35
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	17	0.35
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	17	0.35
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	19	0.34
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	7	0.34
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	7	0.34
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	7	0.34
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	7	0.34
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	7	0.34
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	7	0.34
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	7	0.34
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	18	0.34
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	2	0.34
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	2	0.34
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	5	0.34
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	5	0.34
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	5	0.34
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	5	0.34
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	9	0.34
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	9	0.34
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	16	0.34
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	16	0.34
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	16	0.34
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	16	0.34
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	11	0.34
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	15	0.34
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	15	0.34
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	16	0.34
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	16	0.34
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	16	0.34
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	16	0.34
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	16	0.34
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	16	0.34
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	16	0.34
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	16	0.34
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	16	0.34
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	16	0.34
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	16	0.34
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	1	0.34
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	1	0.34
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	2	0.34
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	2	0.34
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	9	0.34
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	9	0.34
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG12	12	0.34
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG13	12	0.34
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	2	0.34
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	2	0.34
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	7	0.34
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	7	0.34
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	10	0.34
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	10	0.34
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	13	0.34
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	13	0.34
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	2	0.34
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	2	0.34
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	12	0.34
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	12	0.34
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	20	0.34
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	20	0.34
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	20	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	20	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	20	0.34
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	20	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	10	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	10	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	10	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	10	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	10	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	10	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	18	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	18	0.34
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	18	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	18	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	18	0.34
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	18	0.34
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	20	0.34
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	20	0.34
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	20	0.34
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	16	0.34
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	16	0.34
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG2	15	0.34
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG3	15	0.34
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	20	0.34
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	18	0.34
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	3	0.34
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	18	0.34
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	12	0.34
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	12	0.34
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	12	0.34
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	10	0.34
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	19	0.34
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	6	0.34
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	5	0.34
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	5	0.34
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	18	0.34
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	18	0.34
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	3	0.34
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	8	0.34
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	16	0.34
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	16	0.34
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	1	0.34
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	1	0.34
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	3	0.34
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	3	0.34
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	9	0.34
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	20	0.34
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	9	0.34
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	9	0.34
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	12	0.34
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	13	0.34
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	6	0.34
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	19	0.34
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	19	0.34
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	19	0.34
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	2	0.34
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	2	0.34
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	15	0.34
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	1	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	7	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	19	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	19	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	19	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	19	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	19	0.34
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	19	0.34
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	7	0.34
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	4	0.34
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	4	0.34
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	4	0.34
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	11	0.34
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	3	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	5	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	5	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	5	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	11	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	11	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	11	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	15	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	15	0.34
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	15	0.34
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	11	0.34
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	11	0.34
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	11	0.34
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	12	0.34
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	8	0.34
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	8	0.34
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	12	0.34
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	12	0.34
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	12	0.34
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	5	0.34
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	14	0.34
(1,299)	1:33:A:VAL:H	1:83:A:LEU:HA	19	0.34
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	13	0.34
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	5	0.34
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	5	0.34
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	18	0.34
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	3	0.34
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	2	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	13	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	13	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	13	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	14	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	14	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	14	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	17	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	17	0.34
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	17	0.34
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	1	0.34
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	1	0.34
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	1	0.34
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	1	0.34
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	1	0.34
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	1	0.34
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	5	0.34
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	15	0.34
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	4	0.34
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	4	0.34
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	4	0.34
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	9	0.34
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	9	0.34
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	9	0.34
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	15	0.34
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	15	0.34
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	15	0.34
(1,191)	1:25:A:THR:H	1:37:A:THR:H	17	0.34
(1,181)	1:23:A:LYS:HD3	1:24:A:SER:H	2	0.34
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	2	0.34
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	7	0.34
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	3	0.34
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	3	0.34
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	3	0.34
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	10	0.34
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	18	0.34
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	4	0.34
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	4	0.34
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	11	0.34
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	11	0.34
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	11	0.34
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	12	0.34
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	14	0.34
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	1	0.34
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	1	0.34
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	2	0.34
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	2	0.34
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	7	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	2	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	2	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	9	0.34
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	9	0.34
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	3	0.34
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	8	0.34
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	10	0.33
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	14	0.33
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	19	0.33
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	10	0.33
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	10	0.33
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	10	0.33
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	14	0.33
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	14	0.33
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	14	0.33
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	14	0.33
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	14	0.33
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	14	0.33
(2,81)	1:30:A:HIS:HD1	1:31:A:HIS:HD1	9	0.33
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	14	0.33
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	14	0.33
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	14	0.33
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	14	0.33
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	14	0.33
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	14	0.33
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	13	0.33
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	7	0.33
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	3	0.33
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	15	0.33
(1,1113)	1:12:A:THR:HA	1:84:A:HIS:HD2	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	2	0.33
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	2	0.33
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	2	0.33
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	2	0.33
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	7	0.33
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	7	0.33
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	7	0.33
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	7	0.33
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	2	0.33
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	2	0.33
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	2	0.33
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	2	0.33
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	13	0.33
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	13	0.33
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	13	0.33
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	13	0.33
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	14	0.33
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	14	0.33
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	19	0.33
(1,1003)	1:11:A:TYR:HD1	1:33:A:VAL:HA	11	0.33
(1,1003)	1:11:A:TYR:HD2	1:33:A:VAL:HA	11	0.33
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD11	3	0.33
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD12	3	0.33
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD13	3	0.33
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD11	3	0.33
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD12	3	0.33
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD13	3	0.33
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	12	0.33
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	12	0.33
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	12	0.33
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	5	0.33
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	5	0.33
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	5	0.33
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	5	0.33
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	5	0.33
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	5	0.33
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	8	0.33
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	8	0.33
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	8	0.33
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	8	0.33
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	1	0.33
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	1	0.33
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	12	0.33
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	12	0.33
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	12	0.33
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	1	0.33
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	1	0.33
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	12	0.33
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	14	0.33
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	9	0.33
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	11	0.33
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	11	0.33
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	11	0.33
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	2	0.33
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	2	0.33
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	2	0.33
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	6	0.33
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	15	0.33
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	16	0.33
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	4	0.33
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	6	0.33
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	17	0.33
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	16	0.33
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	16	0.33
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	5	0.33
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	16	0.33
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	14	0.33
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	6	0.33
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	6	0.33
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	17	0.33
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	17	0.33
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	12	0.33
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	10	0.33
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	5	0.33
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	2	0.33
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	3	0.33
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	19	0.33
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	19	0.33
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	13	0.33
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	17	0.33
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	5	0.33
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	15	0.33
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	1	0.33
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	4	0.33
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	4	0.33
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	4	0.33
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	9	0.33
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	9	0.33
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	9	0.33
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	2	0.33
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	14	0.33
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	14	0.33
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	4	0.33
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	5	0.33
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	5	0.33
(1,505)	1:53:A:GLN:H	1:61:A:ASN:HD22	6	0.33
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	1	0.33
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	13	0.33
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	9	0.33
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	9	0.33
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	9	0.33
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	19	0.33
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	19	0.33
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	19	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	12	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	12	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	12	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	17	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	17	0.33
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	17	0.33
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	18	0.33
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	18	0.33
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	1	0.33
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	1	0.33
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	18	0.33
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	18	0.33
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	6	0.33
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	1	0.33
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	1	0.33
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	1	0.33
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	6	0.33
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	8	0.33
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	3	0.33
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	9	0.33
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	2	0.33
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	11	0.33
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	11	0.33
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	11	0.33
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	1	0.33
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	13	0.33
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	7	0.33
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	16	0.33
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	16	0.33
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	11	0.33
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	4	0.33
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	10	0.33
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	13	0.33
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	11	0.33
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	11	0.33
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	11	0.33
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	5	0.33
(1,181)	1:23:A:LYS:HD3	1:24:A:SER:H	7	0.33
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	12	0.33
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	10	0.33
(1,137)	1:20:A:LYS:HD2	1:21:A:ASP:H	3	0.33
(1,137)	1:20:A:LYS:HD3	1:21:A:ASP:H	3	0.33
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	9	0.33
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	9	0.33
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	17	0.33
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	10	0.33
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	10	0.33
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	10	0.33
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	20	0.33
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	20	0.33
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	20	0.33
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	6	0.33
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	15	0.33
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	9	0.33
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	13	0.33
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	3	0.33
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	3	0.33
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	19	0.33
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	9	0.33
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	16	0.33
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	6	0.33
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	3	0.33
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	3	0.33
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	1	0.33
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	6	0.33
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	2	0.32
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	9	0.32
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	7	0.32
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	7	0.32
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG11	12	0.32
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG12	12	0.32
(2,77)	1:26:A:TRP:HE3	1:33:A:VAL:HG13	12	0.32
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	5	0.32
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	5	0.32
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	5	0.32
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	5	0.32
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	5	0.32
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	5	0.32
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	10	0.32
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	10	0.32
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	10	0.32
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	10	0.32
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	10	0.32
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	10	0.32
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	9	0.32
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	9	0.32
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	5	0.32
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	13	0.32
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	20	0.32
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	14	0.32
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	14	0.32
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	14	0.32
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	16	0.32
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	16	0.32
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	16	0.32
(2,14)	1:21:A:ASP:H	1:51:A:ARG:HE	4	0.32
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	11	0.32
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	17	0.32
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	17	0.32
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	16	0.32
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	16	0.32
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	20	0.32
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	20	0.32
(1,1102)	1:39:A:PHE:HD1	1:75:A:SER:HA	4	0.32
(1,1102)	1:39:A:PHE:HD2	1:75:A:SER:HA	4	0.32
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	13	0.32
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	13	0.32
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	20	0.32
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	20	0.32
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	3	0.32
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	7	0.32
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	13	0.32
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	3	0.32
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	3	0.32
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	3	0.32
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	3	0.32
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	3	0.32
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	3	0.32
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	3	0.32
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	19	0.32
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	19	0.32
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	3	0.32
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	3	0.32
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	17	0.32
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	17	0.32
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	12	0.32
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	12	0.32
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	12	0.32
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	12	0.32
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	12	0.32
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	12	0.32
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	3	0.32
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	3	0.32
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	11	0.32
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	11	0.32
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	7	0.32
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	7	0.32
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	8	0.32
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	4	0.32
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	4	0.32
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	1	0.32
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	1	0.32
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	11	0.32
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	11	0.32
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	10	0.32
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	10	0.32
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	17	0.32
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	15	0.32
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	16	0.32
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	6	0.32
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	12	0.32
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	3	0.32
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	3	0.32
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	3	0.32
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	15	0.32
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	15	0.32
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	15	0.32
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	16	0.32
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	16	0.32
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	16	0.32
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	20	0.32
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	20	0.32
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	20	0.32
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	3	0.32
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	3	0.32
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	5	0.32
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	5	0.32
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	4	0.32
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	2	0.32
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	5	0.32
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	8	0.32
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	20	0.32
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	15	0.32
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	19	0.32
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	8	0.32
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	1	0.32
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	12	0.32
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	9	0.32
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	9	0.32
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	16	0.32
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	3	0.32
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	3	0.32
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	16	0.32
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	3	0.32
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	3	0.32
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	17	0.32
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	20	0.32
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	7	0.32
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	7	0.32
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	7	0.32
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	16	0.32
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	18	0.32
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	1	0.32
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	1	0.32
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	1	0.32
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	6	0.32
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	6	0.32
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	6	0.32
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	11	0.32
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	5	0.32
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	16	0.32
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	20	0.32
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	20	0.32
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	10	0.32
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	17	0.32
(1,549)	1:59:A:THR:HA	1:61:A:ASN:H	8	0.32
(1,540)	1:30:A:HIS:H	1:59:A:THR:H	5	0.32
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	9	0.32
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	6	0.32
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	6	0.32
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	6	0.32
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	18	0.32
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	2	0.32
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	2	0.32
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	3	0.32
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	3	0.32
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	3	0.32
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	13	0.32
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	13	0.32
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	18	0.32
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	13	0.32
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	15	0.32
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	11	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	9	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	9	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	9	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	20	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	20	0.32
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	20	0.32
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	7	0.32
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	18	0.32
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	13	0.32
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	15	0.32
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	1	0.32
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	6	0.32
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	6	0.32
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	3	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	9	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	9	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	9	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	18	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	18	0.32
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	18	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	9	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	9	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	9	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	9	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	9	0.32
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	9	0.32
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	7	0.32
(1,191)	1:25:A:THR:H	1:37:A:THR:H	12	0.32
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	10	0.32
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	10	0.32
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	2	0.32
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	17	0.32
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	17	0.32
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	13	0.32
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	13	0.32
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	6	0.32
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	6	0.32
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	15	0.32
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	7	0.32
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	8	0.32
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	13	0.32
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	19	0.32
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	14	0.32
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	17	0.32
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	19	0.32
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	1	0.31
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB2	19	0.31
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB3	19	0.31
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	18	0.31
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	18	0.31
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	12	0.31
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	12	0.31
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	2	0.31
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	4	0.31
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	9	0.31
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	9	0.31
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE1	12	0.31
(1,1105)	1:77:A:LYS:HE2	1:78:A:TYR:HE2	12	0.31
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE1	12	0.31
(1,1105)	1:77:A:LYS:HE3	1:78:A:TYR:HE2	12	0.31
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	11	0.31
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	11	0.31
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	11	0.31
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	11	0.31
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	8	0.31
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	8	0.31
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	1	0.31
(1,1076)	1:43:A:TRP:HD1	1:74:A:LEU:HG	9	0.31
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	18	0.31
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	11	0.31
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	11	0.31
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	11	0.31
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	11	0.31
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	11	0.31
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	11	0.31
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	2	0.31
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	2	0.31
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	16	0.31
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	16	0.31
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	16	0.31
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	16	0.31
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	16	0.31
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	16	0.31
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	20	0.31
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	20	0.31
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	4	0.31
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	1	0.31
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	20	0.31
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	9	0.31
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	9	0.31
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	20	0.31
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	20	0.31
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	13	0.31
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	13	0.31
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	13	0.31
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	4	0.31
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	4	0.31
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	16	0.31
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	16	0.31
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	16	0.31
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	3	0.31
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	4	0.31
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	2	0.31
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	2	0.31
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	18	0.31
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	18	0.31
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	2	0.31
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	2	0.31
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	8	0.31
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	8	0.31
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	8	0.31
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	12	0.31
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	13	0.31
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	2	0.31
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	19	0.31
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	6	0.31
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	12	0.31
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	17	0.31
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	17	0.31
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	17	0.31
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	2	0.31
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	3	0.31
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	11	0.31
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	10	0.31
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	12	0.31
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	16	0.31
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	18	0.31
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	19	0.31
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	10	0.31
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	11	0.31
(1,770)	1:81:A:GLY:HA3	1:83:A:LEU:H	16	0.31
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	19	0.31
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	1	0.31
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	1	0.31
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	1	0.31
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	6	0.31
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	3	0.31
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	3	0.31
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	3	0.31
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	5	0.31
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	5	0.31
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	10	0.31
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	10	0.31
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	4	0.31
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	1	0.31
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	11	0.31
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	7	0.31
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	7	0.31
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	8	0.31
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	8	0.31
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	19	0.31
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	12	0.31
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	18	0.31
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	10	0.31
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	1	0.31
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	14	0.31
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	14	0.31
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	10	0.31
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	3	0.31
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	5	0.31
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	6	0.31
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	12	0.31
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	14	0.31
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	3	0.31
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	9	0.31
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	4	0.31
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	15	0.31
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	1	0.31
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	18	0.31
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	8	0.31
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	1	0.31
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	1	0.31
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	13	0.31
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	1	0.31
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	1	0.31
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	1	0.31
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	3	0.31
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	2	0.31
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	2	0.31
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	10	0.31
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	5	0.31
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	19	0.31
(1,235)	1:28:A:ILE:H	1:55:A:GLY:HA3	2	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	3	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	3	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	3	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	8	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	8	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	8	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	11	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	11	0.31
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	11	0.31
(1,227)	1:28:A:ILE:H	1:83:A:LEU:HG	19	0.31
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	3	0.31
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	3	0.31
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	3	0.31
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	10	0.31
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	10	0.31
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	5	0.31
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	5	0.31
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	5	0.31
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	4	0.31
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	4	0.31
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	3	0.31
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	4	0.31
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	10	0.31
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	15	0.31
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	10	0.31
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	7	0.31
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	7	0.31
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	4	0.31
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	11	0.31
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE2	1	0.31
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE3	1	0.31
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	12	0.31
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	12	0.31
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	12	0.31
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	19	0.31
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	15	0.31
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	15	0.31
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	16	0.31
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	16	0.31
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	8	0.31
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	8	0.31
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	18	0.31
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	18	0.31
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	10	0.31
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	12	0.31
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	16	0.3
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	17	0.3
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	14	0.3
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	16	0.3
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	10	0.3
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	10	0.3
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	2	0.3
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	2	0.3
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	2	0.3
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	2	0.3
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	2	0.3
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	19	0.3
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	19	0.3
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	19	0.3
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	19	0.3
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	19	0.3
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	19	0.3
(2,66)	1:90:A:LYS:HA	1:93:A:LYS:H	16	0.3
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	8	0.3
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	14	0.3
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	1	0.3
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	9	0.3
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	9	0.3
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	19	0.3
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	19	0.3
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	12	0.3
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	1	0.3
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	15	0.3
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	6	0.3
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	6	0.3
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	6	0.3
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	7	0.3
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	7	0.3
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	14	0.3
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	14	0.3
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	14	0.3
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	8	0.3
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	8	0.3
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	17	0.3
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	17	0.3
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	17	0.3
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	17	0.3
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	4	0.3
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	20	0.3
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	12	0.3
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	14	0.3
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	5	0.3
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	5	0.3
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	5	0.3
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	5	0.3
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	17	0.3
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	17	0.3
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	17	0.3
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	17	0.3
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	17	0.3
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	17	0.3
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	17	0.3
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	17	0.3
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	17	0.3
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	17	0.3
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	17	0.3
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	8	0.3
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	8	0.3
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	19	0.3
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	19	0.3
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	19	0.3
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	19	0.3
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	19	0.3
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	19	0.3
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	15	0.3
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	15	0.3
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	19	0.3
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	19	0.3
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	13	0.3
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	13	0.3
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	12	0.3
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	12	0.3
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	12	0.3
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	12	0.3
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	12	0.3
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	12	0.3
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	12	0.3
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	12	0.3
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	12	0.3
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	12	0.3
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	12	0.3
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	12	0.3
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	18	0.3
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	18	0.3
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	18	0.3
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	12	0.3
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	6	0.3
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	6	0.3
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	20	0.3
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	20	0.3
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	20	0.3
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	20	0.3
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB2	15	0.3
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB3	15	0.3
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	15	0.3
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	3	0.3
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	15	0.3
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	4	0.3
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	16	0.3
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	17	0.3
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	5	0.3
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	8	0.3
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	15	0.3
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	8	0.3
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	8	0.3
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	8	0.3
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	3	0.3
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	19	0.3
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	19	0.3
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	19	0.3
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	5	0.3
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	7	0.3
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	13	0.3
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	1	0.3
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	13	0.3
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	3	0.3
(1,779)	1:10:A:TYR:HA	1:84:A:HIS:H	5	0.3
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	5	0.3
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	18	0.3
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	10	0.3
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	10	0.3
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	11	0.3
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	2	0.3
(1,736)	1:33:A:VAL:HB	1:81:A:GLY:H	19	0.3
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	17	0.3
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	16	0.3
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	16	0.3
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	15	0.3
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	15	0.3
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	6	0.3
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	6	0.3
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	6	0.3
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	1	0.3
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	6	0.3
(1,577)	1:61:A:ASN:HA	1:64:A:ASP:H	3	0.3
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	1	0.3
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	1	0.3
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	19	0.3
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	18	0.3
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	4	0.3
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	10	0.3
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	12	0.3
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	17	0.3
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	1	0.3
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	2	0.3
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	20	0.3
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	1	0.3
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	2	0.3
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	15	0.3
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	18	0.3
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	9	0.3
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	5	0.3
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	17	0.3
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	8	0.3
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	6	0.3
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	16	0.3
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	17	0.3
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	18	0.3
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	18	0.3
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	8	0.3
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	15	0.3
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	1	0.3
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	18	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	1	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	1	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	1	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	10	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	10	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	12	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	12	0.3
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	12	0.3
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	14	0.3
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	14	0.3
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	14	0.3
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	13	0.3
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	13	0.3
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	13	0.3
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	1	0.3
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	10	0.3
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	11	0.3
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	19	0.3
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	3	0.3
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	3	0.3
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	3	0.3
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	6	0.3
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	6	0.3
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	6	0.3
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	8	0.3
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	8	0.3
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	8	0.3
(1,174)	1:21:A:ASP:HB2	1:24:A:SER:H	17	0.3
(1,174)	1:21:A:ASP:HB3	1:24:A:SER:H	17	0.3
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	11	0.3
(1,164)	1:23:A:LYS:H	1:23:A:LYS:HD3	11	0.3
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	6	0.3
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	11	0.3
(1,88)	1:13:A:LEU:HB2	1:14:A:GLU:H	13	0.3
(1,88)	1:13:A:LEU:HB3	1:14:A:GLU:H	13	0.3
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	2	0.3
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	2	0.3
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	2	0.3
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	2	0.3
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	7	0.3
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	7	0.3
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	20	0.3
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	20	0.3
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	20	0.3
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	18	0.3
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	18	0.3
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	15	0.29
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	3	0.29
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	3	0.29
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	4	0.29
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	20	0.29
(3,24)	1:37:A:THR:O	1:41:A:GLU:H	16	0.29
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	19	0.29
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	20	0.29
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	5	0.29
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	5	0.29
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	17	0.29
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	18	0.29
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	18	0.29
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	18	0.29
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	3	0.29
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	16	0.29
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	6	0.29
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	11	0.29
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	12	0.29
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	18	0.29
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	18	0.29
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	18	0.29
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	17	0.29
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	17	0.29
(1,1115)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	14	0.29
(1,1115)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	14	0.29
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	12	0.29
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	12	0.29
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	12	0.29
(1,1103)	1:34:A:TYR:HD1	1:75:A:SER:HA	12	0.29
(1,1103)	1:34:A:TYR:HD2	1:75:A:SER:HA	12	0.29
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	17	0.29
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	17	0.29
(1,1088)	1:61:A:ASN:HD21	1:62:A:PHE:HA	19	0.29
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	2	0.29
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	8	0.29
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	8	0.29
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	8	0.29
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	8	0.29
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	8	0.29
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	8	0.29
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	8	0.29
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	8	0.29
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	8	0.29
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	8	0.29
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	8	0.29
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	10	0.29
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	10	0.29
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	13	0.29
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	13	0.29
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	13	0.29
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	13	0.29
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	13	0.29
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	13	0.29
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	16	0.29
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	16	0.29
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	9	0.29
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	9	0.29
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	1	0.29
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	1	0.29
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	3	0.29
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	3	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	4	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	4	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	4	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	4	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	4	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	4	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	13	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	13	0.29
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	13	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	13	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	13	0.29
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	13	0.29
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	18	0.29
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	18	0.29
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	18	0.29
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	18	0.29
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	16	0.29
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	16	0.29
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	3	0.29
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	3	0.29
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	8	0.29
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	2	0.29
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	10	0.29
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	18	0.29
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	17	0.29
(1,888)	1:89:A:SER:HG	1:92:A:ALA:H	5	0.29
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	15	0.29
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	8	0.29
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	10	0.29
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	18	0.29
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	19	0.29
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	5	0.29
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	17	0.29
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG2	4	0.29
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG3	4	0.29
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	11	0.29
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	13	0.29
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	14	0.29
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	8	0.29
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	6	0.29
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	18	0.29
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	18	0.29
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	2	0.29
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	16	0.29
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	14	0.29
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	12	0.29
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	13	0.29
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	15	0.29
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	7	0.29
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	7	0.29
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	2	0.29
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	2	0.29
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	1	0.29
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	1	0.29
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	6	0.29
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	13	0.29
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	7	0.29
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	4	0.29
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	19	0.29
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	11	0.29
(1,603)	1:49:A:VAL:HG21	1:66:A:GLY:H	3	0.29
(1,603)	1:49:A:VAL:HG22	1:66:A:GLY:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:49:A:VAL:HG23	1:66:A:GLY:H	3	0.29
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	8	0.29
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	10	0.29
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	17	0.29
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	7	0.29
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	14	0.29
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	8	0.29
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	19	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	18	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	18	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	18	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	18	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	18	0.29
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	18	0.29
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	2	0.29
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	2	0.29
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	13	0.29
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	14	0.29
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	13	0.29
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	1	0.29
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	8	0.29
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	17	0.29
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	17	0.29
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	4	0.29
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	4	0.29
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	19	0.29
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	19	0.29
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	19	0.29
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	16	0.29
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	16	0.29
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	16	0.29
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	12	0.29
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	12	0.29
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	17	0.29
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	11	0.29
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	8	0.29
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	11	0.29
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	20	0.29
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	11	0.29
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	11	0.29
(1,249)	1:29:A:LEU:H	1:34:A:TYR:HD1	5	0.29
(1,249)	1:29:A:LEU:H	1:34:A:TYR:HD2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	4	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	4	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	4	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	5	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	5	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	5	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	6	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	6	0.29
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	6	0.29
(1,221)	1:16:A:ILE:HD11	1:28:A:ILE:H	2	0.29
(1,221)	1:16:A:ILE:HD12	1:28:A:ILE:H	2	0.29
(1,221)	1:16:A:ILE:HD13	1:28:A:ILE:H	2	0.29
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	9	0.29
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	14	0.29
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	15	0.29
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG2	12	0.29
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG3	12	0.29
(1,164)	1:23:A:LYS:H	1:23:A:LYS:HD3	12	0.29
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	12	0.29
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	13	0.29
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	1	0.29
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	1	0.29
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	1	0.29
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG2	20	0.29
(1,135)	1:21:A:ASP:H	1:23:A:LYS:HG3	20	0.29
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	18	0.29
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	18	0.29
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	18	0.29
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	19	0.29
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	1	0.29
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	15	0.29
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	12	0.29
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	12	0.29
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	12	0.29
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	8	0.29
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	8	0.29
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	8	0.29
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	18	0.29
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	18	0.29
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	18	0.29
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	12	0.29
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	20	0.29
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	11	0.29
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	2	0.29
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	4	0.29
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	10	0.28
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	5	0.28
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	16	0.28
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	4	0.28
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	16	0.28
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	3	0.28
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	3	0.28
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	2	0.28
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	2	0.28
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	2	0.28
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	8	0.28
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	8	0.28
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	8	0.28
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	8	0.28
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	8	0.28
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	8	0.28
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	18	0.28
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	18	0.28
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	18	0.28
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	18	0.28
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	18	0.28
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	18	0.28
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	5	0.28
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	5	0.28
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	13	0.28
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	6	0.28
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	10	0.28
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	14	0.28
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	20	0.28
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	20	0.28
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	6	0.28
(1,1113)	1:12:A:THR:HA	1:84:A:HIS:HD2	20	0.28
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	15	0.28
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	5	0.28
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	8	0.28
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	15	0.28
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	20	0.28
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	4	0.28
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	18	0.28
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	18	0.28
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	18	0.28
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	18	0.28
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	18	0.28
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	18	0.28
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	17	0.28
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	17	0.28
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	5	0.28
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	5	0.28
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	5	0.28
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	6	0.28
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	6	0.28
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	6	0.28
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	6	0.28
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	6	0.28
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	6	0.28
(1,961)	1:10:A:TYR:HD1	1:81:A:GLY:HA2	10	0.28
(1,961)	1:10:A:TYR:HD2	1:81:A:GLY:HA2	10	0.28
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	9	0.28
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	9	0.28
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	9	0.28
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	16	0.28
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	10	0.28
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	13	0.28
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	2	0.28
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	3	0.28
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	18	0.28
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	7	0.28
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	8	0.28
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	9	0.28
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	15	0.28
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	19	0.28
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	8	0.28
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	6	0.28
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	7	0.28
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	8	0.28
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	13	0.28
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	11	0.28
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	3	0.28
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	19	0.28
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	19	0.28
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	13	0.28
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	13	0.28
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	19	0.28
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	19	0.28
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	10	0.28
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	15	0.28
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	16	0.28
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	3	0.28
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	1	0.28
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	1	0.28
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	1	0.28
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	17	0.28
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	17	0.28
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	17	0.28
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	7	0.28
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	7	0.28
(1,721)	1:33:A:VAL:HG21	1:80:A:ILE:H	11	0.28
(1,721)	1:33:A:VAL:HG22	1:80:A:ILE:H	11	0.28
(1,721)	1:33:A:VAL:HG23	1:80:A:ILE:H	11	0.28
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	1	0.28
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE1	7	0.28
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE2	7	0.28
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	17	0.28
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	1	0.28
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	10	0.28
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	4	0.28
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	4	0.28
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	12	0.28
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	9	0.28
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	9	0.28
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	14	0.28
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	4	0.28
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	4	0.28
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	4	0.28
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	11	0.28
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	11	0.28
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	11	0.28
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	11	0.28
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	13	0.28
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	10	0.28
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	10	0.28
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	1	0.28
(1,534)	1:58:A:ALA:H	1:61:A:ASN:HA	9	0.28
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	14	0.28
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	11	0.28
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	2	0.28
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	2	0.28
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	2	0.28
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	11	0.28
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	20	0.28
(1,366)	1:26:A:TRP:HD1	1:37:A:THR:H	1	0.28
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	10	0.28
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	12	0.28
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	9	0.28
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	15	0.28
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	2	0.28
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	7	0.28
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	9	0.28
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD21	19	0.28
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD22	19	0.28
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD23	19	0.28
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	12	0.28
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	14	0.28
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	5	0.28
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	5	0.28
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	5	0.28
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	12	0.28
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	18	0.28
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	4	0.28
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	4	0.28
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	19	0.28
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	2	0.28
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	2	0.28
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	2	0.28
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	13	0.28
(1,191)	1:25:A:THR:H	1:37:A:THR:H	11	0.28
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	5	0.28
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	3	0.28
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	6	0.28
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	7	0.28
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	17	0.28
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	6	0.28
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	6	0.28
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	14	0.28
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	1	0.28
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	13	0.28
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	19	0.28
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	16	0.28
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	20	0.28
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	12	0.28
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	12	0.28
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	4	0.28
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	4	0.28
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	6	0.28
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	4	0.28
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	4	0.28
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	1	0.28
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	10	0.27
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	5	0.27
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	4	0.27
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	12	0.27
(2,88)	1:53:A:GLN:HE22	1:56:A:GLY:HA3	3	0.27
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	16	0.27
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	16	0.27
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	16	0.27
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	16	0.27
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	16	0.27
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	16	0.27
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	20	0.27
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	20	0.27
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	20	0.27
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	20	0.27
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	20	0.27
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	20	0.27
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	8	0.27
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	8	0.27
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	15	0.27
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	20	0.27
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	10	0.27
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	10	0.27
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	20	0.27
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	11	0.27
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	11	0.27
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE1	19	0.27
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE2	19	0.27
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	18	0.27
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	18	0.27
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	18	0.27
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	2	0.27
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	13	0.27
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	13	0.27
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	13	0.27
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	13	0.27
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	13	0.27
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	13	0.27
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	13	0.27
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	19	0.27
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	19	0.27
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	1	0.27
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	1	0.27
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	17	0.27
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	17	0.27
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	17	0.27
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	17	0.27
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	17	0.27
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	17	0.27
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	3	0.27
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	3	0.27
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	5	0.27
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	5	0.27
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	6	0.27
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	6	0.27
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	11	0.27
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	11	0.27
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	18	0.27
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	18	0.27
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	6	0.27
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	6	0.27
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	6	0.27
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	6	0.27
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	6	0.27
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	16	0.27
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	16	0.27
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	16	0.27
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	16	0.27
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	16	0.27
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	16	0.27
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	13	0.27
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	13	0.27
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	13	0.27
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	13	0.27
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	7	0.27
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	7	0.27
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	5	0.27
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	7	0.27
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	14	0.27
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	3	0.27
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	3	0.27
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	9	0.27
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	16	0.27
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	16	0.27
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG2	12	0.27
(1,911)	1:93:A:LYS:H	1:93:A:LYS:HG3	12	0.27
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	11	0.27
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	13	0.27
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	12	0.27
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	16	0.27
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	1	0.27
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	7	0.27
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	7	0.27
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	7	0.27
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	15	0.27
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	15	0.27
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	15	0.27
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	20	0.27
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	6	0.27
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	6	0.27
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	6	0.27
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	3	0.27
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	1	0.27
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	4	0.27
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	17	0.27
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	19	0.27
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	20	0.27
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	7	0.27
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	11	0.27
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	9	0.27
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	7	0.27
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	20	0.27
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	3	0.27
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	7	0.27
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	10	0.27
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	18	0.27
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	11	0.27
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	8	0.27
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	8	0.27
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	8	0.27
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	9	0.27
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	17	0.27
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	3	0.27
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	19	0.27
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	4	0.27
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	4	0.27
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	9	0.27
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	9	0.27
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	4	0.27
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	16	0.27
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	17	0.27
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	17	0.27
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE1	12	0.27
(1,701)	1:78:A:TYR:H	1:78:A:TYR:HE2	12	0.27
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	11	0.27
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	15	0.27
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	1	0.27
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	1	0.27
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	13	0.27
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	3	0.27
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	3	0.27
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	3	0.27
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	16	0.27
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	7	0.27
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	14	0.27
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	14	0.27
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	14	0.27
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	2	0.27
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	20	0.27
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	16	0.27
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	16	0.27
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	8	0.27
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	8	0.27
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	11	0.27
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	11	0.27
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	12	0.27
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	10	0.27
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	7	0.27
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	9	0.27
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	9	0.27
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	7	0.27
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	10	0.27
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	3	0.27
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	5	0.27
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	7	0.27
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	7	0.27
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	7	0.27
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	17	0.27
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	7	0.27
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	13	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	1	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	1	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	3	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	3	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	11	0.27
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	11	0.27
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	10	0.27
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	10	0.27
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	9	0.27
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	9	0.27
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	9	0.27
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	11	0.27
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	11	0.27
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:37:A:THR:HA	1:41:A:GLU:H	12	0.27
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	11	0.27
(1,388)	1:36:A:LEU:HD21	1:39:A:PHE:H	7	0.27
(1,388)	1:36:A:LEU:HD22	1:39:A:PHE:H	7	0.27
(1,388)	1:36:A:LEU:HD23	1:39:A:PHE:H	7	0.27
(1,388)	1:36:A:LEU:HD11	1:39:A:PHE:H	7	0.27
(1,388)	1:36:A:LEU:HD12	1:39:A:PHE:H	7	0.27
(1,388)	1:36:A:LEU:HD13	1:39:A:PHE:H	7	0.27
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD11	20	0.27
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD12	20	0.27
(1,387)	1:39:A:PHE:H	1:40:A:LEU:HD13	20	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	4	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	4	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	4	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	8	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	8	0.27
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	8	0.27
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	20	0.27
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	17	0.27
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	9	0.27
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	20	0.27
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	10	0.27
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	5	0.27
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	18	0.27
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	16	0.27
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	17	0.27
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	13	0.27
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	16	0.27
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	17	0.27
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	4	0.27
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	5	0.27
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	2	0.27
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	15	0.27
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	3	0.27
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	3	0.27
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	4	0.27
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	19	0.27
(1,269)	1:31:A:HIS:H	1:31:A:HIS:HD2	2	0.27
(1,264)	1:30:A:HIS:HD1	1:31:A:HIS:H	16	0.27
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	11	0.27
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	15	0.27
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	19	0.27
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	19	0.27
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	15	0.27
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	2	0.27
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	14	0.27
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	3	0.27
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	15	0.27
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	2	0.27
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	15	0.27
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	5	0.27
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	8	0.27
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	8	0.27
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	8	0.27
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	18	0.27
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	3	0.26
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	16	0.26
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	4	0.26
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	3	0.26
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	20	0.26
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB2	7	0.26
(2,91)	1:61:A:ASN:HD21	1:62:A:PHE:HB3	7	0.26
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	4	0.26
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	4	0.26
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	4	0.26
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	4	0.26
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	4	0.26
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	4	0.26
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	6	0.26
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	8	0.26
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	9	0.26
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	12	0.26
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	7	0.26
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	7	0.26
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	20	0.26
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	20	0.26
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	20	0.26
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	20	0.26
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	10	0.26
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	10	0.26
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	10	0.26
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	2	0.26
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	7	0.26
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	7	0.26
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	4	0.26
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	4	0.26
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD1	11	0.26
(1,1069)	1:39:A:PHE:HE1	1:62:A:PHE:HD2	11	0.26
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD1	11	0.26
(1,1069)	1:39:A:PHE:HE2	1:62:A:PHE:HD2	11	0.26
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	16	0.26
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	16	0.26
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	16	0.26
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	16	0.26
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG21	1:34:A:TYR:HE2	5	0.26
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG22	1:34:A:TYR:HE2	5	0.26
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG23	1:34:A:TYR:HE2	5	0.26
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG11	1:34:A:TYR:HE2	5	0.26
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG12	1:34:A:TYR:HE2	5	0.26
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE1	5	0.26
(1,1055)	1:33:A:VAL:HG13	1:34:A:TYR:HE2	5	0.26
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	19	0.26
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	11	0.26
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	11	0.26
(1,1018)	1:16:A:ILE:HD11	1:26:A:TRP:HE3	19	0.26
(1,1018)	1:16:A:ILE:HD12	1:26:A:TRP:HE3	19	0.26
(1,1018)	1:16:A:ILE:HD13	1:26:A:TRP:HE3	19	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	4	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	4	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	10	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	10	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	14	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	14	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	15	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	15	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	16	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	16	0.26
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	19	0.26
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	15	0.26
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	15	0.26
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	15	0.26
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	20	0.26
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	20	0.26
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	20	0.26
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	20	0.26
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	20	0.26
(1,947)	1:95:A:SER:HA	1:98:A:LEU:H	15	0.26
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	20	0.26
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	4	0.26
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	7	0.26
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	2	0.26
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	18	0.26
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	5	0.26
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	3	0.26
(1,902)	1:91:A:ILE:HG12	1:92:A:ALA:H	9	0.26
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	14	0.26
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	10	0.26
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	10	0.26
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	10	0.26
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	16	0.26
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	17	0.26
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	1	0.26
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	1	0.26
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	6	0.26
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	13	0.26
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	16	0.26
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	3	0.26
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	11	0.26
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	14	0.26
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	5	0.26
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	20	0.26
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	15	0.26
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	7	0.26
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	9	0.26
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	1	0.26
(1,758)	1:11:A:TYR:H	1:82:A:GLU:H	2	0.26
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	5	0.26
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	5	0.26
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	9	0.26
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	16	0.26
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	16	0.26
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	13	0.26
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	18	0.26
(1,744)	1:9:A:LYS:HB2	1:81:A:GLY:H	11	0.26
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	6	0.26
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	12	0.26
(1,721)	1:33:A:VAL:HG21	1:80:A:ILE:H	7	0.26
(1,721)	1:33:A:VAL:HG22	1:80:A:ILE:H	7	0.26
(1,721)	1:33:A:VAL:HG23	1:80:A:ILE:H	7	0.26
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	2	0.26
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	2	0.26
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	2	0.26
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	3	0.26
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	6	0.26
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	12	0.26
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	2	0.26
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	2	0.26
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	2	0.26
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	9	0.26
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	9	0.26
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	9	0.26
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	12	0.26
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	18	0.26
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	18	0.26
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	18	0.26
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	17	0.26
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	15	0.26
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	3	0.26
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	3	0.26
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	4	0.26
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	4	0.26
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	4	0.26
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	4	0.26
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	4	0.26
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	4	0.26
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	12	0.26
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	12	0.26
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	14	0.26
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	2	0.26
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	17	0.26
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	15	0.26
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	9	0.26
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	9	0.26
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	9	0.26
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	16	0.26
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	17	0.26
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	18	0.26
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	5	0.26
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	15	0.26
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	7	0.26
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	15	0.26
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE1	11	0.26
(1,295)	1:33:A:VAL:H	1:34:A:TYR:HE2	11	0.26
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	18	0.26
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	18	0.26
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	11	0.26
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	11	0.26
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	11	0.26
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	1	0.26
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	9	0.26
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	16	0.26
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	12	0.26
(1,258)	1:30:A:HIS:H	1:59:A:THR:H	5	0.26
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	9	0.26
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	9	0.26
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	9	0.26
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG21	20	0.26
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG22	20	0.26
(1,234)	1:28:A:ILE:H	1:28:A:ILE:HG23	20	0.26
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	5	0.26
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	5	0.26
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	5	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	16	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	16	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	16	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	16	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	16	0.26
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	16	0.26
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	8	0.26
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	12	0.26
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	18	0.26
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	8	0.26
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	2	0.26
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	12	0.26
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	20	0.26
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	3	0.26
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	3	0.26
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	3	0.26
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	7	0.26
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	7	0.26
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	7	0.26
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	16	0.26
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	16	0.26
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	16	0.26
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	6	0.26
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	12	0.26
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	6	0.26
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	6	0.26
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	6	0.26
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	9	0.26
(1,75)	1:12:A:THR:HG1	1:13:A:LEU:H	6	0.26
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	5	0.26
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	5	0.26
(1,38)	1:10:A:TYR:H	1:81:A:GLY:HA2	13	0.26
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	7	0.26
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	7	0.26
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	4	0.26
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	11	0.26
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	18	0.26
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	3	0.25
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	4	0.25
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	6	0.25
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	5	0.25
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	17	0.25
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	15	0.25
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	17	0.25
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	17	0.25
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	17	0.25
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	2	0.25
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	10	0.25
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	11	0.25
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	9	0.25
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	19	0.25
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	19	0.25
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	10	0.25
(2,33)	1:51:A:ARG:HD2	1:53:A:GLN:H	3	0.25
(2,33)	1:51:A:ARG:HD3	1:53:A:GLN:H	3	0.25
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	3	0.25
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	10	0.25
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	10	0.25
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	10	0.25
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	10	0.25
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	10	0.25
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	10	0.25
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	13	0.25
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	13	0.25
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	9	0.25
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	9	0.25
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	6	0.25
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	6	0.25
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	16	0.25
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	16	0.25
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	16	0.25
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	16	0.25
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	2	0.25
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	2	0.25
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	11	0.25
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	11	0.25
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	14	0.25
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	14	0.25
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	2	0.25
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	2	0.25
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	2	0.25
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	2	0.25
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	2	0.25
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	2	0.25
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	15	0.25
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	15	0.25
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD1	1	0.25
(1,966)	1:10:A:TYR:HD1	1:11:A:TYR:HD2	1	0.25
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD1	1	0.25
(1,966)	1:10:A:TYR:HD2	1:11:A:TYR:HD2	1	0.25
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	14	0.25
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	20	0.25
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	20	0.25
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB2	14	0.25
(1,921)	1:95:A:SER:H	1:96:A:GLU:HB3	14	0.25
(1,915)	1:94:A:PRO:HB2	1:95:A:SER:H	18	0.25
(1,915)	1:94:A:PRO:HB3	1:95:A:SER:H	18	0.25
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG2	16	0.25
(1,900)	1:92:A:ALA:H	1:93:A:LYS:HG3	16	0.25
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	10	0.25
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	16	0.25
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	2	0.25
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	2	0.25
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	2	0.25
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	6	0.25
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	5	0.25
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	12	0.25
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	15	0.25
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	16	0.25
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	15	0.25
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	17	0.25
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	8	0.25
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	2	0.25
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	17	0.25
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	6	0.25
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	17	0.25
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	19	0.25
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	19	0.25
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	2	0.25
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	2	0.25
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	7	0.25
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	6	0.25
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	6	0.25
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	6	0.25
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	8	0.25
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	8	0.25
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	8	0.25
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	20	0.25
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	20	0.25
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	20	0.25
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	19	0.25
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	19	0.25
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	3	0.25
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	5	0.25
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	8	0.25
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	8	0.25
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	9	0.25
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	9	0.25
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	20	0.25
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	12	0.25
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	18	0.25
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	12	0.25
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	12	0.25
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	7	0.25
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	7	0.25
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	7	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	3	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	10	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	10	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	10	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	10	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	10	0.25
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	10	0.25
(1,562)	1:27:A:VAL:HB	1:62:A:PHE:H	11	0.25
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	1	0.25
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	1	0.25
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	3	0.25
(1,525)	1:57:A:ASP:H	1:61:A:ASN:HD21	20	0.25
(1,520)	1:56:A:GLY:HA3	1:57:A:ASP:H	9	0.25
(1,504)	1:51:A:ARG:HA	1:53:A:GLN:H	9	0.25
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	13	0.25
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	16	0.25
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	16	0.25
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	16	0.25
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	16	0.25
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	20	0.25
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	2	0.25
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	2	0.25
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	2	0.25
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	2	0.25
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	2	0.25
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	10	0.25
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	7	0.25
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	7	0.25
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	16	0.25
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	12	0.25
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	12	0.25
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	12	0.25
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	5	0.25
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD21	9	0.25
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD22	9	0.25
(1,393)	1:40:A:LEU:H	1:50:A:LEU:HD23	9	0.25
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	10	0.25
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	10	0.25
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	10	0.25
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	4	0.25
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	9	0.25
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	8	0.25
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	20	0.25
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	15	0.25
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	16	0.25
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	10	0.25
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	1	0.25
(1,290)	1:32:A:LYS:HE2	1:33:A:VAL:H	8	0.25
(1,290)	1:32:A:LYS:HE3	1:33:A:VAL:H	8	0.25
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	13	0.25
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	13	0.25
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	13	0.25
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	1	0.25
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	1	0.25
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	16	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	11	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	11	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	11	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	13	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	13	0.25
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	13	0.25
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	1	0.25
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	18	0.25
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	11	0.25
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	12	0.25
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	12	0.25
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	20	0.25
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	20	0.25
(1,178)	1:23:A:LYS:HZ1	1:24:A:SER:H	2	0.25
(1,178)	1:23:A:LYS:HZ2	1:24:A:SER:H	2	0.25
(1,178)	1:23:A:LYS:HZ3	1:24:A:SER:H	2	0.25
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	18	0.25
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	18	0.25
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	2	0.25
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	5	0.25
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	11	0.25
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	2	0.25
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	6	0.25
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	3	0.25
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	5	0.25
(1,94)	1:14:A:GLU:H	1:91:A:ILE:HB	5	0.25
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	18	0.25
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	19	0.25
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	19	0.25
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	11	0.25
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	11	0.25
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	11	0.25
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	9	0.25
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	9	0.25
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	8	0.25
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	16	0.25
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	16	0.25
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	17	0.24
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	20	0.24
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	3	0.24
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	7	0.24
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	16	0.24
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	16	0.24
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	16	0.24
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	1	0.24
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	1	0.24
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	1	0.24
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	13	0.24
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	13	0.24
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	9	0.24
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	10	0.24
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	3	0.24
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	3	0.24
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE1	1	0.24
(1,1062)	1:39:A:PHE:HE1	1:78:A:TYR:HE2	1	0.24
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE1	1	0.24
(1,1062)	1:39:A:PHE:HE2	1:78:A:TYR:HE2	1	0.24
(1,1058)	1:39:A:PHE:HD1	1:43:A:TRP:HB2	12	0.24
(1,1058)	1:39:A:PHE:HD1	1:43:A:TRP:HB3	12	0.24
(1,1058)	1:39:A:PHE:HD2	1:43:A:TRP:HB2	12	0.24
(1,1058)	1:39:A:PHE:HD2	1:43:A:TRP:HB3	12	0.24
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	17	0.24
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	17	0.24
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	5	0.24
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	5	0.24
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	5	0.24
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	5	0.24
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	5	0.24
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	5	0.24
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	20	0.24
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	17	0.24
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	17	0.24
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	13	0.24
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	13	0.24
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG21	19	0.24
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG22	19	0.24
(1,999)	1:11:A:TYR:HD1	1:28:A:ILE:HG23	19	0.24
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG21	19	0.24
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG22	19	0.24
(1,999)	1:11:A:TYR:HD2	1:28:A:ILE:HG23	19	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	9	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	9	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	9	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	16	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	16	0.24
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	16	0.24
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	14	0.24
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	14	0.24
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	14	0.24
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	14	0.24
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	14	0.24
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	9	0.24
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	9	0.24
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	13	0.24
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	13	0.24
(1,973)	1:10:A:TYR:HD1	1:84:A:HIS:HD1	14	0.24
(1,973)	1:10:A:TYR:HD2	1:84:A:HIS:HD1	14	0.24
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	16	0.24
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	16	0.24
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	16	0.24
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	5	0.24
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	5	0.24
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	9	0.24
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	9	0.24
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	17	0.24
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	17	0.24
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	11	0.24
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	11	0.24
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	11	0.24
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	9	0.24
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	1	0.24
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	1	0.24
(1,931)	1:95:A:SER:HB3	1:96:A:GLU:H	16	0.24
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	5	0.24
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	3	0.24
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	6	0.24
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	1	0.24
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	3	0.24
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	2	0.24
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	14	0.24
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	6	0.24
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	4	0.24
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	2	0.24
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	17	0.24
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	12	0.24
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	8	0.24
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	9	0.24
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	11	0.24
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	14	0.24
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	4	0.24
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	1	0.24
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:11:A:TYR:H	1:84:A:HIS:H	16	0.24
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	12	0.24
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	12	0.24
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	4	0.24
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	8	0.24
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	13	0.24
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	13	0.24
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	4	0.24
(1,730)	1:11:A:TYR:HE1	1:81:A:GLY:H	5	0.24
(1,730)	1:11:A:TYR:HE2	1:81:A:GLY:H	5	0.24
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	5	0.24
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	5	0.24
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	20	0.24
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	6	0.24
(1,680)	1:75:A:SER:HB2	1:77:A:LYS:H	20	0.24
(1,680)	1:75:A:SER:HB3	1:77:A:LYS:H	20	0.24
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	20	0.24
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	20	0.24
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	19	0.24
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	19	0.24
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	4	0.24
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	4	0.24
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	4	0.24
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	2	0.24
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	20	0.24
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	6	0.24
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	6	0.24
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	20	0.24
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	18	0.24
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	15	0.24
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	2	0.24
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	2	0.24
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	2	0.24
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	13	0.24
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	20	0.24
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	10	0.24
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	1	0.24
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	1	0.24
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	1	0.24
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	20	0.24
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	20	0.24
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	6	0.24
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	5	0.24
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	14	0.24
(1,366)	1:26:A:TRP:HD1	1:37:A:THR:H	3	0.24
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	19	0.24
(1,336)	1:35:A:ASP:H	1:80:A:ILE:H	11	0.24
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	3	0.24
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	17	0.24
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	2	0.24
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	3	0.24
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	5	0.24
(1,276)	1:30:A:HIS:HD1	1:32:A:LYS:H	16	0.24
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	6	0.24
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	7	0.24
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	7	0.24
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	6	0.24
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	18	0.24
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	8	0.24
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	3	0.24
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	3	0.24
(1,175)	1:21:A:ASP:HA	1:24:A:SER:H	17	0.24
(1,171)	1:23:A:LYS:H	1:25:A:THR:HG1	2	0.24
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	17	0.24
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	7	0.24
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	17	0.24
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	11	0.24
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	17	0.24
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	17	0.24
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	17	0.24
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	19	0.24
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE2	13	0.24
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE3	13	0.24
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	7	0.24
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	1	0.24
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	3	0.24
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	3	0.24
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	20	0.24
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	20	0.24
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	14	0.24
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	14	0.24
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	4	0.24
(1,12)	1:4:A:SER:H	1:6:A:LYS:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	2	0.24
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	12	0.24
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	16	0.23
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	16	0.23
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	12	0.23
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	11	0.23
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	20	0.23
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	8	0.23
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	5	0.23
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	5	0.23
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	5	0.23
(2,87)	1:43:A:TRP:HD1	1:67:A:PHE:HB3	15	0.23
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	18	0.23
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	18	0.23
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	18	0.23
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	18	0.23
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	18	0.23
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	18	0.23
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	15	0.23
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	20	0.23
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	7	0.23
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	7	0.23
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	7	0.23
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	17	0.23
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	17	0.23
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	17	0.23
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	13	0.23
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	4	0.23
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	11	0.23
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	11	0.23
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	1	0.23
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	8	0.23
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	1	0.23
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	1	0.23
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	12	0.23
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA2	4	0.23
(1,1098)	1:39:A:PHE:HZ	1:66:A:GLY:HA3	4	0.23
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	8	0.23
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	10	0.23
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	13	0.23
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	5	0.23
(1,1077)	1:43:A:TRP:HE3	1:67:A:PHE:HB3	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:43:A:TRP:HD1	1:74:A:LEU:HG	4	0.23
(1,1076)	1:43:A:TRP:HD1	1:74:A:LEU:HG	12	0.23
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	1	0.23
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	1	0.23
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	1	0.23
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	1	0.23
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	10	0.23
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	10	0.23
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	13	0.23
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	13	0.23
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	2	0.23
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	2	0.23
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	19	0.23
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	19	0.23
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	14	0.23
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	14	0.23
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	14	0.23
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	14	0.23
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	14	0.23
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	14	0.23
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	14	0.23
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	14	0.23
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	14	0.23
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	14	0.23
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	14	0.23
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	14	0.23
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	18	0.23
(1,1016)	1:16:A:ILE:HA	1:26:A:TRP:HE3	5	0.23
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	11	0.23
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	11	0.23
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	11	0.23
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	11	0.23
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	11	0.23
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	11	0.23
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	8	0.23
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	8	0.23
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	7	0.23
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	7	0.23
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	17	0.23
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	4	0.23
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	13	0.23
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	10	0.23
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	19	0.23
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	5	0.23
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	2	0.23
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	10	0.23
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	14	0.23
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	20	0.23
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	2	0.23
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	5	0.23
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	8	0.23
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	7	0.23
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	3	0.23
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	15	0.23
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	3	0.23
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	16	0.23
(1,765)	1:10:A:TYR:HA	1:83:A:LEU:H	5	0.23
(1,759)	1:11:A:TYR:HD1	1:82:A:GLU:H	17	0.23
(1,759)	1:11:A:TYR:HD2	1:82:A:GLU:H	17	0.23
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	11	0.23
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	11	0.23
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	14	0.23
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	20	0.23
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	1	0.23
(1,741)	1:79:A:ILE:HG21	1:81:A:GLY:H	6	0.23
(1,741)	1:79:A:ILE:HG22	1:81:A:GLY:H	6	0.23
(1,741)	1:79:A:ILE:HG23	1:81:A:GLY:H	6	0.23
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	15	0.23
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	15	0.23
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	15	0.23
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	18	0.23
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	11	0.23
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	11	0.23
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	4	0.23
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	4	0.23
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	6	0.23
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	6	0.23
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	6	0.23
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	9	0.23
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	12	0.23
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	4	0.23
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	12	0.23
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	19	0.23
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	8	0.23
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	9	0.23
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	20	0.23
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	20	0.23
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	20	0.23
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE1	11	0.23
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE2	11	0.23
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	4	0.23
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	19	0.23
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	14	0.23
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	4	0.23
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	20	0.23
(1,538)	1:29:A:LEU:HG	1:59:A:THR:H	18	0.23
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	7	0.23
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	7	0.23
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	15	0.23
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	17	0.23
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	17	0.23
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	17	0.23
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	17	0.23
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	17	0.23
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	17	0.23
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	15	0.23
(1,431)	1:39:A:PHE:HA	1:43:A:TRP:H	12	0.23
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	11	0.23
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	4	0.23
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	4	0.23
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	7	0.23
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	8	0.23
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	7	0.23
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	19	0.23
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	6	0.23
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	18	0.23
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	16	0.23
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	20	0.23
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	20	0.23
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	20	0.23
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	1	0.23
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	11	0.23
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	19	0.23
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	2	0.23
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	2	0.23
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	1	0.23
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	6	0.23
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	6	0.23
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	12	0.23
(1,247)	1:29:A:LEU:H	1:34:A:TYR:HE1	6	0.23
(1,247)	1:29:A:LEU:H	1:34:A:TYR:HE2	6	0.23
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	7	0.23
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	9	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	14	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	20	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	20	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	20	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	20	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	20	0.23
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	20	0.23
(1,191)	1:25:A:THR:H	1:37:A:THR:H	14	0.23
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	18	0.23
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	18	0.23
(1,178)	1:23:A:LYS:HZ1	1:24:A:SER:H	5	0.23
(1,178)	1:23:A:LYS:HZ2	1:24:A:SER:H	5	0.23
(1,178)	1:23:A:LYS:HZ3	1:24:A:SER:H	5	0.23
(1,160)	1:21:A:ASP:HB2	1:23:A:LYS:H	13	0.23
(1,160)	1:21:A:ASP:HB3	1:23:A:LYS:H	13	0.23
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	8	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	6	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	6	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	6	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	15	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	15	0.23
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	15	0.23
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	17	0.23
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	2	0.23
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG2	11	0.23
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG3	11	0.23
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	13	0.23
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE2	9	0.23
(1,91)	1:14:A:GLU:H	1:90:A:LYS:HE3	9	0.23
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	5	0.23
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	16	0.23
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	16	0.23
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	16	0.23
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	19	0.23
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	19	0.23
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	19	0.23
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	1	0.23
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	16	0.23
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	5	0.23
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	11	0.23
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	12	0.23
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	5	0.23
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	13	0.23
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	13	0.23
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	2	0.23
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	0.23
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	20	0.23
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	9	0.22
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	2	0.22
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	13	0.22
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	17	0.22
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	9	0.22
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	14	0.22
(2,88)	1:53:A:GLN:HE22	1:56:A:GLY:HA3	9	0.22
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	20	0.22
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	20	0.22
(2,68)	1:94:A:PRO:HG3	1:96:A:GLU:H	18	0.22
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	9	0.22
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	13	0.22
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	13	0.22
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	13	0.22
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	16	0.22
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	16	0.22
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	16	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	6	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	6	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	15	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	16	0.22
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	16	0.22
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	14	0.22
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	12	0.22
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	1	0.22
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	8	0.22
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	8	0.22
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	8	0.22
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	8	0.22
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	17	0.22
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	17	0.22
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	19	0.22
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	19	0.22
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	19	0.22
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	19	0.22
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	19	0.22
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	19	0.22
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	19	0.22
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	19	0.22
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	19	0.22
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	19	0.22
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	19	0.22
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	19	0.22
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	18	0.22
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	18	0.22
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	10	0.22
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	10	0.22
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	18	0.22
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	18	0.22
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	18	0.22
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	18	0.22
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	18	0.22
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	18	0.22
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	2	0.22
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	2	0.22
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	2	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	2	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	2	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	2	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	2	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	2	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	12	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	12	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	12	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	12	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	12	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	12	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	15	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	15	0.22
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	15	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	15	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	15	0.22
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	15	0.22
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA2	5	0.22
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA3	5	0.22
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	10	0.22
(1,930)	1:96:A:GLU:H	1:97:A:THR:HA	17	0.22
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	12	0.22
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	18	0.22
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	17	0.22
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	1	0.22
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	1	0.22
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	19	0.22
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	19	0.22
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	11	0.22
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	5	0.22
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	10	0.22
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	19	0.22
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	19	0.22
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	19	0.22
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	15	0.22
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	15	0.22
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	4	0.22
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	5	0.22
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	12	0.22
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	14	0.22
(1,870)	1:87:A:ASP:HB2	1:91:A:ILE:H	4	0.22
(1,856)	1:89:A:SER:HG	1:90:A:LYS:H	7	0.22
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	7	0.22
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	13	0.22
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	1	0.22
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	9	0.22
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	11	0.22
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	18	0.22
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	19	0.22
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	9	0.22
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	6	0.22
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	7	0.22
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	7	0.22
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	7	0.22
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	13	0.22
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	13	0.22
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	13	0.22
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	15	0.22
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	20	0.22
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	14	0.22
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	20	0.22
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	15	0.22
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	12	0.22
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	12	0.22
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	4	0.22
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	12	0.22
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	2	0.22
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	12	0.22
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	11	0.22
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	13	0.22
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	18	0.22
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	18	0.22
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	9	0.22
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	9	0.22
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	5	0.22
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	19	0.22
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	8	0.22
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	17	0.22
(1,629)	1:62:A:PHE:HD1	1:72:A:ARG:H	8	0.22
(1,629)	1:62:A:PHE:HD2	1:72:A:ARG:H	8	0.22
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	5	0.22
(1,607)	1:65:A:VAL:HG21	1:67:A:PHE:H	2	0.22
(1,607)	1:65:A:VAL:HG22	1:67:A:PHE:H	2	0.22
(1,607)	1:65:A:VAL:HG23	1:67:A:PHE:H	2	0.22
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	10	0.22
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	14	0.22
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	5	0.22
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	5	0.22
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	17	0.22
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	17	0.22
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	17	0.22
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	9	0.22
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	1	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG11	2	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG12	2	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG13	2	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG21	2	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG22	2	0.22
(1,564)	1:62:A:PHE:H	1:65:A:VAL:HG23	2	0.22
(1,563)	1:36:A:LEU:HD21	1:62:A:PHE:H	15	0.22
(1,563)	1:36:A:LEU:HD22	1:62:A:PHE:H	15	0.22
(1,563)	1:36:A:LEU:HD23	1:62:A:PHE:H	15	0.22
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	4	0.22
(1,546)	1:59:A:THR:H	1:59:A:THR:HB	7	0.22
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	18	0.22
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	18	0.22
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	5	0.22
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	5	0.22
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	5	0.22
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	7	0.22
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	11	0.22
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	20	0.22
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD21	7	0.22
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD22	7	0.22
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD23	7	0.22
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	3	0.22
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	6	0.22
(1,433)	1:41:A:GLU:HA	1:43:A:TRP:H	16	0.22
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	8	0.22
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	8	0.22
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	3	0.22
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	3	0.22
(1,419)	1:38:A:LYS:HE3	1:42:A:GLU:H	8	0.22
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	17	0.22
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	17	0.22
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	17	0.22
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	16	0.22
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	2	0.22
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:36:A:LEU:HD11	1:40:A:LEU:H	4	0.22
(1,389)	1:36:A:LEU:HD12	1:40:A:LEU:H	4	0.22
(1,389)	1:36:A:LEU:HD13	1:40:A:LEU:H	4	0.22
(1,388)	1:36:A:LEU:HD21	1:39:A:PHE:H	17	0.22
(1,388)	1:36:A:LEU:HD22	1:39:A:PHE:H	17	0.22
(1,388)	1:36:A:LEU:HD23	1:39:A:PHE:H	17	0.22
(1,388)	1:36:A:LEU:HD11	1:39:A:PHE:H	17	0.22
(1,388)	1:36:A:LEU:HD12	1:39:A:PHE:H	17	0.22
(1,388)	1:36:A:LEU:HD13	1:39:A:PHE:H	17	0.22
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	10	0.22
(1,353)	1:25:A:THR:HB	1:36:A:LEU:H	4	0.22
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	9	0.22
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	14	0.22
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	14	0.22
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	14	0.22
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	12	0.22
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD21	4	0.22
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD22	4	0.22
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD23	4	0.22
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	4	0.22
(1,267)	1:30:A:HIS:HD2	1:31:A:HIS:H	2	0.22
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	19	0.22
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	19	0.22
(1,255)	1:30:A:HIS:H	1:34:A:TYR:HD1	5	0.22
(1,255)	1:30:A:HIS:H	1:34:A:TYR:HD2	5	0.22
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	15	0.22
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	20	0.22
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	7	0.22
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	20	0.22
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	8	0.22
(1,221)	1:16:A:ILE:HD11	1:28:A:ILE:H	13	0.22
(1,221)	1:16:A:ILE:HD12	1:28:A:ILE:H	13	0.22
(1,221)	1:16:A:ILE:HD13	1:28:A:ILE:H	13	0.22
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	2	0.22
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	19	0.22
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	3	0.22
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	16	0.22
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	16	0.22
(1,175)	1:21:A:ASP:HA	1:24:A:SER:H	3	0.22
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	15	0.22
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	6	0.22
(1,159)	1:21:A:ASP:HA	1:23:A:LYS:H	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	9	0.22
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	1	0.22
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	14	0.22
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	11	0.22
(1,100)	1:14:A:GLU:H	1:90:A:LYS:HZ1	11	0.22
(1,100)	1:14:A:GLU:H	1:90:A:LYS:HZ2	11	0.22
(1,100)	1:14:A:GLU:H	1:90:A:LYS:HZ3	11	0.22
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	13	0.22
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	13	0.22
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	13	0.22
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	2	0.22
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	20	0.22
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	11	0.22
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	14	0.22
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	14	0.22
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	17	0.22
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	15	0.22
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE2	15	0.22
(1,18)	1:6:A:LYS:H	1:6:A:LYS:HE3	15	0.22
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	14	0.22
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	14	0.22
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	6	0.22
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	14	0.21
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	1	0.21
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	1	0.21
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	1	0.21
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	7	0.21
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	8	0.21
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	18	0.21
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	5	0.21
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	5	0.21
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	12	0.21
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	12	0.21
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	9	0.21
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	10	0.21
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	10	0.21
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	10	0.21
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	4	0.21
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	4	0.21
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	13	0.21
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	6	0.21
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	2	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	2	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	2	0.21
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	3	0.21
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	3	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	3	0.21
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	3	0.21
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	10	0.21
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	10	0.21
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	7	0.21
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	7	0.21
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	3	0.21
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	3	0.21
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	8	0.21
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	8	0.21
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	3	0.21
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	3	0.21
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	4	0.21
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	4	0.21
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA2	17	0.21
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA3	17	0.21
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	6	0.21
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	6	0.21
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	6	0.21
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	18	0.21
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	18	0.21
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	18	0.21
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	2	0.21
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	18	0.21
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	2	0.21
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	6	0.21
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	3	0.21
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	3	0.21
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	3	0.21
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	7	0.21
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	9	0.21
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	9	0.21
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	18	0.21
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	18	0.21
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	19	0.21
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	2	0.21
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	14	0.21
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	11	0.21
(1,824)	1:84:A:HIS:HA	1:88:A:ARG:H	11	0.21
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	1	0.21
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	8	0.21
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG2	3	0.21
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG3	3	0.21
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG2	7	0.21
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG3	7	0.21
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	6	0.21
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	9	0.21
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	10	0.21
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	17	0.21
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	20	0.21
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	17	0.21
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	17	0.21
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	1	0.21
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	4	0.21
(1,778)	1:84:A:HIS:H	1:84:A:HIS:HD2	20	0.21
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	15	0.21
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	15	0.21
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	13	0.21
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	20	0.21
(1,765)	1:10:A:TYR:HA	1:83:A:LEU:H	19	0.21
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	4	0.21
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	4	0.21
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	1	0.21
(1,745)	1:80:A:ILE:H	1:81:A:GLY:H	17	0.21
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	15	0.21
(1,741)	1:79:A:ILE:HG21	1:81:A:GLY:H	7	0.21
(1,741)	1:79:A:ILE:HG22	1:81:A:GLY:H	7	0.21
(1,741)	1:79:A:ILE:HG23	1:81:A:GLY:H	7	0.21
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	5	0.21
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	19	0.21
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	14	0.21
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	17	0.21
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	12	0.21
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	13	0.21
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	4	0.21
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	4	0.21
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	15	0.21
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	3	0.21
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	4	0.21
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	4	0.21
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	5	0.21
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	6	0.21
(1,649)	1:73:A:GLU:HG2	1:75:A:SER:H	2	0.21
(1,649)	1:73:A:GLU:HG3	1:75:A:SER:H	2	0.21
(1,640)	1:69:A:THR:HB	1:72:A:ARG:H	10	0.21
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	7	0.21
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD1	11	0.21
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD2	11	0.21
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	2	0.21
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	20	0.21
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	20	0.21
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	20	0.21
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	13	0.21
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	4	0.21
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	4	0.21
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	11	0.21
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	13	0.21
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	11	0.21
(1,520)	1:56:A:GLY:HA3	1:57:A:ASP:H	19	0.21
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	8	0.21
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	19	0.21
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	8	0.21
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	8	0.21
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	8	0.21
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	10	0.21
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	8	0.21
(1,454)	1:46:A:GLY:H	1:47:A:GLU:H	9	0.21
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	15	0.21
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	15	0.21
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	7	0.21
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	7	0.21
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	7	0.21
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	13	0.21
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	13	0.21
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	13	0.21
(1,406)	1:38:A:LYS:HA	1:41:A:GLU:H	19	0.21
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	17	0.21
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	7	0.21
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	7	0.21
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	15	0.21
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	14	0.21
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	16	0.21
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	18	0.21
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	12	0.21
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	18	0.21
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	18	0.21
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	18	0.21
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	19	0.21
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	4	0.21
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	15	0.21
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	9	0.21
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	12	0.21
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	12	0.21
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	9	0.21
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	9	0.21
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	9	0.21
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	15	0.21
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	15	0.21
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	15	0.21
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	17	0.21
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	17	0.21
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	17	0.21
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	20	0.21
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	20	0.21
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	20	0.21
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	17	0.21
(1,259)	1:30:A:HIS:H	1:83:A:LEU:H	2	0.21
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	11	0.21
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	13	0.21
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	14	0.21
(1,214)	1:27:A:VAL:H	1:36:A:LEU:HG	11	0.21
(1,191)	1:25:A:THR:H	1:37:A:THR:H	4	0.21
(1,191)	1:25:A:THR:H	1:37:A:THR:H	8	0.21
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	1	0.21
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	16	0.21
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	15	0.21
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	15	0.21
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	15	0.21
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	18	0.21
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	16	0.21
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	2	0.21
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	2	0.21
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	2	0.21
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	14	0.21
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	14	0.21
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	14	0.21
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	8	0.21
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	14	0.21
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	13	0.21
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG21	18	0.21
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG22	18	0.21
(1,48)	1:11:A:TYR:H	1:12:A:THR:HG23	18	0.21
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	18	0.21
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	5	0.21
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	5	0.21
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	2	0.2
(2,94)	1:84:A:HIS:HB3	1:90:A:LYS:HZ1	19	0.2
(2,94)	1:84:A:HIS:HB3	1:90:A:LYS:HZ2	19	0.2
(2,94)	1:84:A:HIS:HB3	1:90:A:LYS:HZ3	19	0.2
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	20	0.2
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	20	0.2
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	20	0.2
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	20	0.2
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	20	0.2
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	20	0.2
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	6	0.2
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	6	0.2
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	6	0.2
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	8	0.2
(2,60)	1:86:A:ASP:H	1:89:A:SER:HB3	15	0.2
(2,55)	1:34:A:TYR:HB3	1:81:A:GLY:H	18	0.2
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	5	0.2
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	5	0.2
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	5	0.2
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	4	0.2
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	4	0.2
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	4	0.2
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	12	0.2
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	8	0.2
(2,43)	1:39:A:PHE:HZ	1:76:A:LYS:H	9	0.2
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	1	0.2
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	1	0.2
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	8	0.2
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	8	0.2
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	5	0.2
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	5	0.2
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	15	0.2
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	15	0.2
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	2	0.2
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	2	0.2
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	3	0.2
(1,1118)	1:87:A:ASP:HB3	1:90:A:LYS:HZ1	11	0.2
(1,1118)	1:87:A:ASP:HB3	1:90:A:LYS:HZ2	11	0.2
(1,1118)	1:87:A:ASP:HB3	1:90:A:LYS:HZ3	11	0.2
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	16	0.2
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	16	0.2
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	18	0.2
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	7	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	6	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	6	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	6	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	6	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	6	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	6	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	9	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	9	0.2
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	9	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	9	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	9	0.2
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	9	0.2
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	14	0.2
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	14	0.2
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	12	0.2
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	12	0.2
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	6	0.2
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	6	0.2
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	13	0.2
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	13	0.2
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	8	0.2
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	17	0.2
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	17	0.2
(1,1001)	1:11:A:TYR:HD1	1:33:A:VAL:HB	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:11:A:TYR:HD2	1:33:A:VAL:HB	12	0.2
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	6	0.2
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	6	0.2
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	17	0.2
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	17	0.2
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	17	0.2
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	17	0.2
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	17	0.2
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	17	0.2
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	14	0.2
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	14	0.2
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	7	0.2
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	7	0.2
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	7	0.2
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	12	0.2
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	12	0.2
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	12	0.2
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	17	0.2
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	17	0.2
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	17	0.2
(1,967)	1:10:A:TYR:HD1	1:84:A:HIS:HA	5	0.2
(1,967)	1:10:A:TYR:HD2	1:84:A:HIS:HA	5	0.2
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD1	14	0.2
(1,960)	1:9:A:LYS:HA	1:10:A:TYR:HD2	14	0.2
(1,948)	1:96:A:GLU:HA	1:98:A:LEU:H	7	0.2
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	12	0.2
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	12	0.2
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	9	0.2
(1,930)	1:96:A:GLU:H	1:97:A:THR:HA	11	0.2
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	6	0.2
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	14	0.2
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	12	0.2
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	16	0.2
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	7	0.2
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	8	0.2
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	17	0.2
(1,868)	1:13:A:LEU:HB2	1:91:A:ILE:H	13	0.2
(1,868)	1:13:A:LEU:HB3	1:91:A:ILE:H	13	0.2
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	4	0.2
(1,826)	1:87:A:ASP:H	1:88:A:ARG:H	20	0.2
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	13	0.2
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	19	0.2
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	1	0.2
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	13	0.2
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	15	0.2
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	4	0.2
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	6	0.2
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	2	0.2
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	12	0.2
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	13	0.2
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	18	0.2
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	19	0.2
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	20	0.2
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	20	0.2
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	9	0.2
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	9	0.2
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	9	0.2
(1,788)	1:12:A:THR:HA	1:84:A:HIS:H	14	0.2
(1,784)	1:13:A:LEU:H	1:84:A:HIS:H	4	0.2
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	10	0.2
(1,783)	1:12:A:THR:HB	1:84:A:HIS:H	19	0.2
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	13	0.2
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	12	0.2
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	1	0.2
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	1	0.2
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	3	0.2
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	3	0.2
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	15	0.2
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	15	0.2
(1,731)	1:32:A:LYS:HD2	1:81:A:GLY:H	8	0.2
(1,731)	1:32:A:LYS:HD3	1:81:A:GLY:H	8	0.2
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	18	0.2
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	17	0.2
(1,705)	1:35:A:ASP:HB2	1:79:A:ILE:H	5	0.2
(1,705)	1:35:A:ASP:HB3	1:79:A:ILE:H	5	0.2
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	13	0.2
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	19	0.2
(1,678)	1:77:A:LYS:H	1:77:A:LYS:HE2	15	0.2
(1,678)	1:77:A:LYS:H	1:77:A:LYS:HE3	15	0.2
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	2	0.2
(1,659)	1:75:A:SER:H	1:78:A:TYR:HB2	19	0.2
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	11	0.2
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	13	0.2
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	13	0.2
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	13	0.2
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	15	0.2
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	6	0.2
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	15	0.2
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	3	0.2
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	3	0.2
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	3	0.2
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	3	0.2
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	17	0.2
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	17	0.2
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	12	0.2
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	12	0.2
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	15	0.2
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	17	0.2
(1,493)	1:50:A:LEU:HA	1:52:A:GLU:H	11	0.2
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	10	0.2
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	10	0.2
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	10	0.2
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	9	0.2
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	16	0.2
(1,434)	1:40:A:LEU:HB2	1:43:A:TRP:H	10	0.2
(1,434)	1:40:A:LEU:HB3	1:43:A:TRP:H	10	0.2
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	17	0.2
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	17	0.2
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	6	0.2
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	6	0.2
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	6	0.2
(1,404)	1:38:A:LYS:HE3	1:41:A:GLU:H	12	0.2
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	14	0.2
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	19	0.2
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	6	0.2
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	16	0.2
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	15	0.2
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	15	0.2
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	15	0.2
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD21	9	0.2
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD22	9	0.2
(1,313)	1:34:A:TYR:H	1:36:A:LEU:HD23	9	0.2
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	3	0.2
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:32:A:LYS:HD2	1:33:A:VAL:H	8	0.2
(1,291)	1:32:A:LYS:HD3	1:33:A:VAL:H	8	0.2
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	13	0.2
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	18	0.2
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	2	0.2
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	7	0.2
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	12	0.2
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	12	0.2
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	12	0.2
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	15	0.2
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	15	0.2
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	15	0.2
(1,178)	1:23:A:LYS:HZ1	1:24:A:SER:H	4	0.2
(1,178)	1:23:A:LYS:HZ2	1:24:A:SER:H	4	0.2
(1,178)	1:23:A:LYS:HZ3	1:24:A:SER:H	4	0.2
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	5	0.2
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	5	0.2
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	7	0.2
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	10	0.2
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	10	0.2
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	10	0.2
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	6	0.2
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	13	0.2
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	8	0.2
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	15	0.2
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	14	0.2
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	15	0.2
(1,84)	1:12:A:THR:HG21	1:14:A:GLU:H	9	0.2
(1,84)	1:12:A:THR:HG22	1:14:A:GLU:H	9	0.2
(1,84)	1:12:A:THR:HG23	1:14:A:GLU:H	9	0.2
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	9	0.2
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	4	0.2
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	9	0.2
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	6	0.2
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	6	0.2
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	8	0.2
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	8	0.2
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	7	0.2
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	7	0.2
(1,34)	1:3:A:GLN:HG3	1:10:A:TYR:H	3	0.2
(1,26)	1:8:A:VAL:H	1:81:A:GLY:HA2	17	0.2
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD2	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD3	16	0.2
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	13	0.2
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	9	0.2
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	9	0.2
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	3	0.19
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	10	0.19
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	16	0.19
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	18	0.19
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	6	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	10	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	10	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	10	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	13	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	13	0.19
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	13	0.19
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	13	0.19
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	18	0.19
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	20	0.19
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	1	0.19
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	10	0.19
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	10	0.19
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	10	0.19
(2,35)	1:29:A:LEU:HA	1:62:A:PHE:H	15	0.19
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	16	0.19
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	4	0.19
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	4	0.19
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	4	0.19
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	8	0.19
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	8	0.19
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	19	0.19
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	19	0.19
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	9	0.19
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	9	0.19
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	7	0.19
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	7	0.19
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	17	0.19
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	17	0.19
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	16	0.19
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	16	0.19
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	19	0.19
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	19	0.19
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	8	0.19
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	8	0.19
(1,1042)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	8	0.19
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	8	0.19
(1,1042)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	8	0.19
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD1	19	0.19
(1,1038)	1:28:A:ILE:HB	1:34:A:TYR:HD2	19	0.19
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	8	0.19
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	8	0.19
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	10	0.19
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	10	0.19
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	5	0.19
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	5	0.19
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	4	0.19
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	4	0.19
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	4	0.19
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	4	0.19
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	4	0.19
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	4	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	4	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	4	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	4	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG21	19	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG22	19	0.19
(1,995)	1:11:A:TYR:HA	1:80:A:ILE:HG23	19	0.19
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG21	19	0.19
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG22	19	0.19
(1,990)	1:11:A:TYR:HE1	1:33:A:VAL:HG23	19	0.19
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG21	19	0.19
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG22	19	0.19
(1,990)	1:11:A:TYR:HE2	1:33:A:VAL:HG23	19	0.19
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG11	12	0.19
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG12	12	0.19
(1,988)	1:11:A:TYR:HE1	1:33:A:VAL:HG13	12	0.19
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG11	12	0.19
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG12	12	0.19
(1,988)	1:11:A:TYR:HE2	1:33:A:VAL:HG13	12	0.19
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	12	0.19
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	12	0.19
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	12	0.19
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	12	0.19
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	15	0.19
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	5	0.19
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	5	0.19
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	5	0.19
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	20	0.19
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	20	0.19
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG11	14	0.19
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG12	14	0.19
(1,952)	1:5:A:ASP:HA	1:8:A:VAL:HG13	14	0.19
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	8	0.19
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	8	0.19
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	4	0.19
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	4	0.19
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	14	0.19
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	14	0.19
(1,932)	1:95:A:SER:HG	1:96:A:GLU:H	15	0.19
(1,925)	1:94:A:PRO:HG2	1:96:A:GLU:H	2	0.19
(1,920)	1:94:A:PRO:HG2	1:95:A:SER:H	16	0.19
(1,920)	1:94:A:PRO:HG3	1:95:A:SER:H	16	0.19
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	1	0.19
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	3	0.19
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	15	0.19
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	5	0.19
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	14	0.19
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	14	0.19
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	14	0.19
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	3	0.19
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	6	0.19
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	2	0.19
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	2	0.19
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	2	0.19
(1,869)	1:13:A:LEU:HD21	1:91:A:ILE:H	18	0.19
(1,869)	1:13:A:LEU:HD22	1:91:A:ILE:H	18	0.19
(1,869)	1:13:A:LEU:HD23	1:91:A:ILE:H	18	0.19
(1,858)	1:89:A:SER:HB2	1:90:A:LYS:H	9	0.19
(1,858)	1:89:A:SER:HB3	1:90:A:LYS:H	9	0.19
(1,858)	1:89:A:SER:HB2	1:90:A:LYS:H	11	0.19
(1,858)	1:89:A:SER:HB3	1:90:A:LYS:H	11	0.19
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	12	0.19
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	7	0.19
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	4	0.19
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:86:A:ASP:H	1:87:A:ASP:H	20	0.19
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	16	0.19
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	10	0.19
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	16	0.19
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	8	0.19
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	8	0.19
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	8	0.19
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	5	0.19
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	11	0.19
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	17	0.19
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	10	0.19
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	10	0.19
(1,754)	1:10:A:TYR:HB3	1:82:A:GLU:H	19	0.19
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	5	0.19
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	10	0.19
(1,719)	1:34:A:TYR:HB3	1:80:A:ILE:H	11	0.19
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	7	0.19
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	2	0.19
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	20	0.19
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	20	0.19
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	15	0.19
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	8	0.19
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	20	0.19
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	10	0.19
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	10	0.19
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	10	0.19
(1,607)	1:65:A:VAL:HG21	1:67:A:PHE:H	7	0.19
(1,607)	1:65:A:VAL:HG22	1:67:A:PHE:H	7	0.19
(1,607)	1:65:A:VAL:HG23	1:67:A:PHE:H	7	0.19
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	11	0.19
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	13	0.19
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	18	0.19
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	12	0.19
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	12	0.19
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	12	0.19
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	15	0.19
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	15	0.19
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	8	0.19
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	10	0.19
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	10	0.19
(1,574)	1:60:A:GLU:HA	1:64:A:ASP:H	3	0.19
(1,567)	1:60:A:GLU:H	1:62:A:PHE:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	18	0.19
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	9	0.19
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	19	0.19
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	19	0.19
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	19	0.19
(1,542)	1:58:A:ALA:HB1	1:59:A:THR:H	19	0.19
(1,542)	1:58:A:ALA:HB2	1:59:A:THR:H	19	0.19
(1,542)	1:58:A:ALA:HB3	1:59:A:THR:H	19	0.19
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	20	0.19
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	20	0.19
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	12	0.19
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	5	0.19
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	17	0.19
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	19	0.19
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	20	0.19
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	20	0.19
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	20	0.19
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	20	0.19
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	20	0.19
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	20	0.19
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	16	0.19
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	16	0.19
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	5	0.19
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	6	0.19
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	3	0.19
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	3	0.19
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	3	0.19
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	6	0.19
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	5	0.19
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	5	0.19
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	5	0.19
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	11	0.19
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	17	0.19
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	7	0.19
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	2	0.19
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	20	0.19
(1,322)	1:34:A:TYR:HB3	1:35:A:ASP:H	15	0.19
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	1	0.19
(1,314)	1:29:A:LEU:HD21	1:34:A:TYR:H	11	0.19
(1,314)	1:29:A:LEU:HD22	1:34:A:TYR:H	11	0.19
(1,314)	1:29:A:LEU:HD23	1:34:A:TYR:H	11	0.19
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	3	0.19
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	3	0.19
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	5	0.19
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	5	0.19
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	5	0.19
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	14	0.19
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	14	0.19
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	14	0.19
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	18	0.19
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	18	0.19
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	18	0.19
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	20	0.19
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	10	0.19
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	18	0.19
(1,233)	1:13:A:LEU:HD11	1:28:A:ILE:H	5	0.19
(1,233)	1:13:A:LEU:HD12	1:28:A:ILE:H	5	0.19
(1,233)	1:13:A:LEU:HD13	1:28:A:ILE:H	5	0.19
(1,233)	1:13:A:LEU:HD21	1:28:A:ILE:H	5	0.19
(1,233)	1:13:A:LEU:HD22	1:28:A:ILE:H	5	0.19
(1,233)	1:13:A:LEU:HD23	1:28:A:ILE:H	5	0.19
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	2	0.19
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	2	0.19
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	2	0.19
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	5	0.19
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	5	0.19
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	5	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	10	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	10	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	10	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	14	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	14	0.19
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	14	0.19
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	2	0.19
(1,178)	1:23:A:LYS:HZ1	1:24:A:SER:H	14	0.19
(1,178)	1:23:A:LYS:HZ2	1:24:A:SER:H	14	0.19
(1,178)	1:23:A:LYS:HZ3	1:24:A:SER:H	14	0.19
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	6	0.19
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	6	0.19
(1,173)	1:23:A:LYS:HG2	1:24:A:SER:H	18	0.19
(1,173)	1:23:A:LYS:HG3	1:24:A:SER:H	18	0.19
(1,170)	1:23:A:LYS:H	1:37:A:THR:HG1	6	0.19
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	6	0.19
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	6	0.19
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	8	0.19
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	12	0.19
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	19	0.19
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	5	0.19
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	1	0.19
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	1	0.19
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	5	0.19
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	5	0.19
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	5	0.19
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	1	0.19
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	7	0.19
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	13	0.19
(1,99)	1:14:A:GLU:H	1:87:A:ASP:HB2	5	0.19
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	15	0.19
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	10	0.19
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	8	0.19
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	8	0.19
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	2	0.19
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	2	0.19
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	5	0.19
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	5	0.19
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	9	0.19
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	9	0.19
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	15	0.19
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	17	0.19
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	10	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	2	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	2	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	2	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	2	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	2	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	2	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	8	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	8	0.18
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	8	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	8	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	8	0.18
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	8	0.18
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	3	0.18
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:37:A:THR:O	1:41:A:GLU:N	12	0.18
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	10	0.18
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	19	0.18
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	5	0.18
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	6	0.18
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	1	0.18
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	17	0.18
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	17	0.18
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG2	18	0.18
(2,10)	1:16:A:ILE:H	1:17:A:GLN:HG3	18	0.18
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	2	0.18
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	2	0.18
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	10	0.18
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	10	0.18
(1,1081)	1:53:A:GLN:HE22	1:64:A:ASP:HB3	5	0.18
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD1	5	0.18
(1,1068)	1:39:A:PHE:HE1	1:78:A:TYR:HD2	5	0.18
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD1	5	0.18
(1,1068)	1:39:A:PHE:HE2	1:78:A:TYR:HD2	5	0.18
(1,1047)	1:34:A:TYR:HD1	1:77:A:LYS:HA	9	0.18
(1,1047)	1:34:A:TYR:HD2	1:77:A:LYS:HA	9	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	4	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	4	0.18
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	4	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	4	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	4	0.18
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	4	0.18
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	4	0.18
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	4	0.18
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	4	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	4	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	4	0.18
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	4	0.18
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	7	0.18
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	7	0.18
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	10	0.18
(1,1023)	1:24:A:SER:HA	1:26:A:TRP:HZ2	17	0.18
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	16	0.18
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	3	0.18
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	3	0.18
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	5	0.18
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	3	0.18
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	3	0.18
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	3	0.18
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	3	0.18
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	3	0.18
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	3	0.18
(1,989)	1:11:A:TYR:HE1	1:80:A:ILE:HG21	1	0.18
(1,989)	1:11:A:TYR:HE1	1:80:A:ILE:HG22	1	0.18
(1,989)	1:11:A:TYR:HE1	1:80:A:ILE:HG23	1	0.18
(1,989)	1:11:A:TYR:HE2	1:80:A:ILE:HG21	1	0.18
(1,989)	1:11:A:TYR:HE2	1:80:A:ILE:HG22	1	0.18
(1,989)	1:11:A:TYR:HE2	1:80:A:ILE:HG23	1	0.18
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	2	0.18
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	2	0.18
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	2	0.18
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	15	0.18
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	15	0.18
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	15	0.18
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	16	0.18
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	16	0.18
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	18	0.18
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	18	0.18
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	18	0.18
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	18	0.18
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	12	0.18
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	6	0.18
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	6	0.18
(1,919)	1:95:A:SER:H	1:96:A:GLU:HA	10	0.18
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	3	0.18
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	1	0.18
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	18	0.18
(1,883)	1:89:A:SER:HA	1:91:A:ILE:H	1	0.18
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	6	0.18
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	19	0.18
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	3	0.18
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	9	0.18
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	15	0.18
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	3	0.18
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	16	0.18
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	5	0.18
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	4	0.18
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	18	0.18
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	2	0.18
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	2	0.18
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	1	0.18
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	1	0.18
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	3	0.18
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	10	0.18
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	20	0.18
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	20	0.18
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	5	0.18
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	5	0.18
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	20	0.18
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	6	0.18
(1,631)	1:62:A:PHE:HE1	1:72:A:ARG:H	1	0.18
(1,631)	1:62:A:PHE:HE2	1:72:A:ARG:H	1	0.18
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	10	0.18
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE1	5	0.18
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE2	5	0.18
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	10	0.18
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	15	0.18
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	15	0.18
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	15	0.18
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	14	0.18
(1,562)	1:27:A:VAL:HB	1:62:A:PHE:H	3	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	15	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	15	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	15	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	18	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	18	0.18
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	18	0.18
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	1	0.18
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	15	0.18
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	15	0.18
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	19	0.18
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	19	0.18
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	2	0.18
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	13	0.18
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD21	16	0.18
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD22	16	0.18
(1,465)	1:49:A:VAL:H	1:50:A:LEU:HD23	16	0.18
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	10	0.18
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	13	0.18
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	13	0.18
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	15	0.18
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	15	0.18
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD21	4	0.18
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD22	4	0.18
(1,413)	1:41:A:GLU:H	1:50:A:LEU:HD23	4	0.18
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	18	0.18
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	18	0.18
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	18	0.18
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	11	0.18
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	18	0.18
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	18	0.18
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	18	0.18
(1,388)	1:36:A:LEU:HD21	1:39:A:PHE:H	16	0.18
(1,388)	1:36:A:LEU:HD22	1:39:A:PHE:H	16	0.18
(1,388)	1:36:A:LEU:HD23	1:39:A:PHE:H	16	0.18
(1,388)	1:36:A:LEU:HD11	1:39:A:PHE:H	16	0.18
(1,388)	1:36:A:LEU:HD12	1:39:A:PHE:H	16	0.18
(1,388)	1:36:A:LEU:HD13	1:39:A:PHE:H	16	0.18
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	18	0.18
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	6	0.18
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	4	0.18
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	8	0.18
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	6	0.18
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	7	0.18
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	14	0.18
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	14	0.18
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	14	0.18
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	6	0.18
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	17	0.18
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	16	0.18
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	16	0.18
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	16	0.18
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	16	0.18
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	5	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	7	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	7	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	7	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	7	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	7	0.18
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	15	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	6	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	6	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	6	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	8	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	8	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	8	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ1	16	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ2	16	0.18
(1,167)	1:23:A:LYS:H	1:23:A:LYS:HZ3	16	0.18
(1,164)	1:23:A:LYS:H	1:23:A:LYS:HD3	10	0.18
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	17	0.18
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	17	0.18
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	17	0.18
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	10	0.18
(1,141)	1:21:A:ASP:H	1:25:A:THR:HA	14	0.18
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	19	0.18
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	19	0.18
(1,137)	1:20:A:LYS:HD2	1:21:A:ASP:H	19	0.18
(1,137)	1:20:A:LYS:HD3	1:21:A:ASP:H	19	0.18
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	20	0.18
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	4	0.18
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	4	0.18
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	11	0.18
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	11	0.18
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	16	0.18
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	16	0.18
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	11	0.18
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	7	0.18
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD2	10	0.18
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD3	10	0.18
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	1	0.18
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	10	0.18
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	13	0.17
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	17	0.17
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	8	0.17
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	9	0.17
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD2	9	0.17
(2,93)	1:10:A:TYR:HA	1:85:A:PRO:HD3	9	0.17
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	14	0.17
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	14	0.17
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	14	0.17
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	14	0.17
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	14	0.17
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	6	0.17
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	4	0.17
(2,49)	1:11:A:TYR:HD1	1:80:A:ILE:H	11	0.17
(2,49)	1:11:A:TYR:HD2	1:80:A:ILE:H	11	0.17
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	5	0.17
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	5	0.17
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	5	0.17
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	8	0.17
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	8	0.17
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	8	0.17
(2,8)	1:15:A:GLU:H	1:87:A:ASP:HB2	5	0.17
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	18	0.17
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	18	0.17
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	11	0.17
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	14	0.17
(1,1082)	1:53:A:GLN:HE22	1:61:A:ASN:HD22	4	0.17
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB2	6	0.17
(1,1080)	1:53:A:GLN:HE22	1:57:A:ASP:HB3	6	0.17
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	2	0.17
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	12	0.17
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	1	0.17
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	1	0.17
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	15	0.17
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	15	0.17
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	5	0.17
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	5	0.17
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	7	0.17
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	7	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	15	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	15	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	15	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	15	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	15	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	15	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	16	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	16	0.17
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	16	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	16	0.17
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	16	0.17
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE1	20	0.17
(1,975)	1:9:A:LYS:HD2	1:11:A:TYR:HE2	20	0.17
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE1	20	0.17
(1,975)	1:9:A:LYS:HD3	1:11:A:TYR:HE2	20	0.17
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	6	0.17
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	6	0.17
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	6	0.17
(1,968)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	13	0.17
(1,968)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	13	0.17
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	7	0.17
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	6	0.17
(1,909)	1:89:A:SER:HA	1:93:A:LYS:H	17	0.17
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	4	0.17
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	4	0.17
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	11	0.17
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	6	0.17
(1,884)	1:91:A:ILE:H	1:93:A:LYS:H	10	0.17
(1,866)	1:90:A:LYS:H	1:92:A:ALA:HA	19	0.17
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	3	0.17
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	17	0.17
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	10	0.17
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	4	0.17
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	15	0.17
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	11	0.17
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	12	0.17
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	9	0.17
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	14	0.17
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	10	0.17
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	4	0.17
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	12	0.17
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	7	0.17
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	8	0.17
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	15	0.17
(1,780)	1:11:A:TYR:H	1:84:A:HIS:H	12	0.17
(1,779)	1:10:A:TYR:HA	1:84:A:HIS:H	18	0.17
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	2	0.17
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	2	0.17
(1,775)	1:28:A:ILE:HB	1:83:A:LEU:H	19	0.17
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	10	0.17
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	2	0.17
(1,763)	1:29:A:LEU:HD21	1:83:A:LEU:H	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:29:A:LEU:HD22	1:83:A:LEU:H	12	0.17
(1,763)	1:29:A:LEU:HD23	1:83:A:LEU:H	12	0.17
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	9	0.17
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	9	0.17
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	3	0.17
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	18	0.17
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	13	0.17
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	2	0.17
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	16	0.17
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	12	0.17
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	12	0.17
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	12	0.17
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	19	0.17
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	8	0.17
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	8	0.17
(1,698)	1:34:A:TYR:HB3	1:78:A:TYR:H	7	0.17
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	15	0.17
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	12	0.17
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	12	0.17
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	17	0.17
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	11	0.17
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	11	0.17
(1,673)	1:34:A:TYR:HD1	1:77:A:LYS:H	14	0.17
(1,673)	1:34:A:TYR:HD2	1:77:A:LYS:H	14	0.17
(1,661)	1:62:A:PHE:HE1	1:75:A:SER:H	1	0.17
(1,661)	1:62:A:PHE:HE2	1:75:A:SER:H	1	0.17
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG2	15	0.17
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG3	15	0.17
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	3	0.17
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	16	0.17
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	1	0.17
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	17	0.17
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	17	0.17
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	17	0.17
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	18	0.17
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	4	0.17
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	11	0.17
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	17	0.17
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	1	0.17
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	1	0.17
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	2	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	6	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	6	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	9	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	9	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	9	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	10	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	10	0.17
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	10	0.17
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	17	0.17
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	15	0.17
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	13	0.17
(1,453)	1:46:A:GLY:H	1:47:A:GLU:HA	7	0.17
(1,434)	1:40:A:LEU:HB2	1:43:A:TRP:H	11	0.17
(1,434)	1:40:A:LEU:HB3	1:43:A:TRP:H	11	0.17
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	7	0.17
(1,418)	1:41:A:GLU:H	1:47:A:GLU:HA	19	0.17
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	9	0.17
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	9	0.17
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	9	0.17
(1,395)	1:38:A:LYS:HE3	1:40:A:LEU:H	16	0.17
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	14	0.17
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	14	0.17
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	14	0.17
(1,388)	1:36:A:LEU:HD21	1:39:A:PHE:H	14	0.17
(1,388)	1:36:A:LEU:HD22	1:39:A:PHE:H	14	0.17
(1,388)	1:36:A:LEU:HD23	1:39:A:PHE:H	14	0.17
(1,388)	1:36:A:LEU:HD11	1:39:A:PHE:H	14	0.17
(1,388)	1:36:A:LEU:HD12	1:39:A:PHE:H	14	0.17
(1,388)	1:36:A:LEU:HD13	1:39:A:PHE:H	14	0.17
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD21	19	0.17
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD22	19	0.17
(1,386)	1:39:A:PHE:H	1:50:A:LEU:HD23	19	0.17
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	5	0.17
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	10	0.17
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	14	0.17
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	5	0.17
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	3	0.17
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	1	0.17
(1,343)	1:26:A:TRP:HD1	1:36:A:LEU:H	14	0.17
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	17	0.17
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	17	0.17
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	8	0.17
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	1	0.17
(1,323)	1:35:A:ASP:H	1:79:A:ILE:HB	11	0.17
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	9	0.17
(1,318)	1:33:A:VAL:HG21	1:34:A:TYR:H	4	0.17
(1,318)	1:33:A:VAL:HG22	1:34:A:TYR:H	4	0.17
(1,318)	1:33:A:VAL:HG23	1:34:A:TYR:H	4	0.17
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	15	0.17
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	17	0.17
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	6	0.17
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	6	0.17
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	6	0.17
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	6	0.17
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	7	0.17
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	7	0.17
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	7	0.17
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	8	0.17
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	14	0.17
(1,264)	1:30:A:HIS:HD1	1:31:A:HIS:H	18	0.17
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	16	0.17
(1,245)	1:29:A:LEU:H	1:33:A:VAL:HA	11	0.17
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	16	0.17
(1,221)	1:16:A:ILE:HD11	1:28:A:ILE:H	1	0.17
(1,221)	1:16:A:ILE:HD12	1:28:A:ILE:H	1	0.17
(1,221)	1:16:A:ILE:HD13	1:28:A:ILE:H	1	0.17
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	8	0.17
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	8	0.17
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	8	0.17
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	1	0.17
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	19	0.17
(1,196)	1:26:A:TRP:H	1:55:A:GLY:HA2	19	0.17
(1,175)	1:21:A:ASP:HA	1:24:A:SER:H	10	0.17
(1,174)	1:21:A:ASP:HB2	1:24:A:SER:H	12	0.17
(1,174)	1:21:A:ASP:HB3	1:24:A:SER:H	12	0.17
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	3	0.17
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	14	0.17
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	6	0.17
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	6	0.17
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	6	0.17
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	11	0.17
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	11	0.17
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	9	0.17
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	18	0.17
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	4	0.17
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	16	0.17
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	2	0.17
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	1	0.17
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	1	0.17
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	12	0.17
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	12	0.17
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD1	18	0.17
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD2	18	0.17
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	5	0.17
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	9	0.17
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	1	0.17
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	19	0.17
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	10	0.17
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	10	0.17
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	14	0.17
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	4	0.17
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	12	0.17
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	1	0.16
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	9	0.16
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	9	0.16
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	9	0.16
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	6	0.16
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	6	0.16
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	6	0.16
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	6	0.16
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	6	0.16
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	6	0.16
(2,63)	1:90:A:LYS:H	1:93:A:LYS:H	6	0.16
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	14	0.16
(2,40)	1:67:A:PHE:H	1:70:A:ASP:H	14	0.16
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB2	18	0.16
(2,39)	1:67:A:PHE:H	1:68:A:SER:HB3	18	0.16
(2,34)	1:53:A:GLN:HE22	1:57:A:ASP:H	3	0.16
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	2	0.16
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ1	17	0.16
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ2	17	0.16
(1,1119)	1:86:A:ASP:HA	1:90:A:LYS:HZ3	17	0.16
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	20	0.16
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	20	0.16
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	20	0.16
(1,1095)	1:39:A:PHE:HE1	1:62:A:PHE:HA	10	0.16
(1,1095)	1:39:A:PHE:HE2	1:62:A:PHE:HA	10	0.16
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	1	0.16
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	18	0.16
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	11	0.16
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	16	0.16
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	16	0.16
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	16	0.16
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	16	0.16
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	4	0.16
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	4	0.16
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	4	0.16
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	4	0.16
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	4	0.16
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	4	0.16
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	4	0.16
(1,1017)	1:16:A:ILE:HG12	1:26:A:TRP:HE3	2	0.16
(1,1008)	1:26:A:TRP:HA	1:26:A:TRP:HD1	19	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	6	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	6	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	6	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	6	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	6	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	6	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	8	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	8	0.16
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	8	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	8	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	8	0.16
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	8	0.16
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	7	0.16
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	7	0.16
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	7	0.16
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	7	0.16
(1,981)	1:11:A:TYR:HE1	1:16:A:ILE:HG13	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:11:A:TYR:HE2	1:16:A:ILE:HG13	12	0.16
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	3	0.16
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	3	0.16
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	3	0.16
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	19	0.16
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	19	0.16
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG2	20	0.16
(1,916)	1:95:A:SER:H	1:96:A:GLU:HG3	20	0.16
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	9	0.16
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	9	0.16
(1,905)	1:91:A:ILE:HB	1:93:A:LYS:H	19	0.16
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	4	0.16
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	2	0.16
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	19	0.16
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	3	0.16
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	13	0.16
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	20	0.16
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	2	0.16
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	6	0.16
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	16	0.16
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	3	0.16
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	7	0.16
(1,818)	1:87:A:ASP:H	1:89:A:SER:HB3	4	0.16
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG2	2	0.16
(1,817)	1:87:A:ASP:H	1:88:A:ARG:HG3	2	0.16
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	1	0.16
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	14	0.16
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	17	0.16
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	17	0.16
(1,784)	1:13:A:LEU:H	1:84:A:HIS:H	20	0.16
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	9	0.16
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	14	0.16
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	14	0.16
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	6	0.16
(1,743)	1:81:A:GLY:H	1:82:A:GLU:HB3	20	0.16
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	18	0.16
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	18	0.16
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	18	0.16
(1,727)	1:78:A:TYR:HA	1:80:A:ILE:H	19	0.16
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	7	0.16
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	11	0.16
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	8	0.16
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	14	0.16
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	3	0.16
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	3	0.16
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	12	0.16
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	4	0.16
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	15	0.16
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	17	0.16
(1,659)	1:75:A:SER:H	1:78:A:TYR:HB2	1	0.16
(1,655)	1:75:A:SER:H	1:75:A:SER:HB2	19	0.16
(1,655)	1:75:A:SER:H	1:75:A:SER:HB3	19	0.16
(1,648)	1:71:A:ALA:HA	1:75:A:SER:H	6	0.16
(1,632)	1:63:A:GLU:HG2	1:72:A:ARG:H	15	0.16
(1,632)	1:63:A:GLU:HG3	1:72:A:ARG:H	15	0.16
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	6	0.16
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	14	0.16
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	5	0.16
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	5	0.16
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	5	0.16
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD1	17	0.16
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD2	17	0.16
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	12	0.16
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	17	0.16
(1,590)	1:49:A:VAL:HG21	1:65:A:VAL:H	10	0.16
(1,590)	1:49:A:VAL:HG22	1:65:A:VAL:H	10	0.16
(1,590)	1:49:A:VAL:HG23	1:65:A:VAL:H	10	0.16
(1,577)	1:61:A:ASN:HA	1:64:A:ASP:H	4	0.16
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	20	0.16
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	17	0.16
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	17	0.16
(1,565)	1:58:A:ALA:HA	1:62:A:PHE:H	11	0.16
(1,547)	1:59:A:THR:H	1:60:A:GLU:HB2	1	0.16
(1,547)	1:59:A:THR:H	1:60:A:GLU:HB3	1	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	3	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	3	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	3	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	13	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	13	0.16
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	13	0.16
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	15	0.16
(1,518)	1:55:A:GLY:HA3	1:57:A:ASP:H	2	0.16
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	16	0.16
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	16	0.16
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	18	0.16
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	18	0.16
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	18	0.16
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	6	0.16
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	9	0.16
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	15	0.16
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	6	0.16
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	6	0.16
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	6	0.16
(1,377)	1:36:A:LEU:HB2	1:38:A:LYS:H	14	0.16
(1,377)	1:36:A:LEU:HB3	1:38:A:LYS:H	14	0.16
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	2	0.16
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	6	0.16
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	8	0.16
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	13	0.16
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	19	0.16
(1,367)	1:26:A:TRP:HA	1:37:A:THR:H	19	0.16
(1,363)	1:24:A:SER:HA	1:37:A:THR:H	5	0.16
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	8	0.16
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	11	0.16
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	1	0.16
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	2	0.16
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	5	0.16
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	9	0.16
(1,322)	1:34:A:TYR:HB3	1:35:A:ASP:H	13	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	6	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	6	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	9	0.16
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	9	0.16
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	19	0.16
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	20	0.16
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	9	0.16
(1,272)	1:31:A:HIS:H	1:31:A:HIS:HB3	16	0.16
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	7	0.16
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	13	0.16
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	13	0.16
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	12	0.16
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	17	0.16
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	3	0.16
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	3	0.16
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	4	0.16
(1,175)	1:21:A:ASP:HA	1:24:A:SER:H	12	0.16
(1,171)	1:23:A:LYS:H	1:25:A:THR:HG1	19	0.16
(1,152)	1:22:A:SER:H	1:23:A:LYS:H	12	0.16
(1,142)	1:21:A:ASP:H	1:24:A:SER:HA	12	0.16
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	3	0.16
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	3	0.16
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	16	0.16
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	16	0.16
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	20	0.16
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	20	0.16
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG2	10	0.16
(1,128)	1:19:A:HIS:H	1:20:A:LYS:HG3	10	0.16
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	5	0.16
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	15	0.16
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	1	0.16
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	1	0.16
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	1	0.16
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	12	0.16
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	1	0.16
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	1	0.16
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	20	0.16
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	20	0.16
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	6	0.16
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	8	0.16
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	13	0.16
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	15	0.16
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	15	0.16
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	9	0.15
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	5	0.15
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	9	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	5	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	5	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	5	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	5	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	5	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	5	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	12	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	12	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	12	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	12	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	12	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	15	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	15	0.15
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	15	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	15	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	15	0.15
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	15	0.15
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	3	0.15
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	3	0.15
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	3	0.15
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	6	0.15
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	6	0.15
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	8	0.15
(2,46)	1:34:A:TYR:HB2	1:78:A:TYR:H	3	0.15
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	11	0.15
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	17	0.15
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	17	0.15
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	17	0.15
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	14	0.15
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	14	0.15
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	1	0.15
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	6	0.15
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	17	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	13	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	13	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	13	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	13	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	13	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	13	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	20	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	20	0.15
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	20	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	20	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	20	0.15
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	20	0.15
(1,1049)	1:34:A:TYR:HD1	1:75:A:SER:HG	11	0.15
(1,1049)	1:34:A:TYR:HD2	1:75:A:SER:HG	11	0.15
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	18	0.15
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	18	0.15
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	18	0.15
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	18	0.15
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	18	0.15
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	18	0.15
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	18	0.15
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	18	0.15
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	18	0.15
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	18	0.15
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	18	0.15
(1,1033)	1:30:A:HIS:HD2	1:88:A:ARG:HG2	1	0.15
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	20	0.15
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	20	0.15
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	9	0.15
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	9	0.15
(1,1022)	1:25:A:THR:HG21	1:26:A:TRP:HE3	10	0.15
(1,1022)	1:25:A:THR:HG22	1:26:A:TRP:HE3	10	0.15
(1,1022)	1:25:A:THR:HG23	1:26:A:TRP:HE3	10	0.15
(1,1016)	1:16:A:ILE:HA	1:26:A:TRP:HE3	2	0.15
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	15	0.15
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	15	0.15
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD11	11	0.15
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD12	11	0.15
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD13	11	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD11	11	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD12	11	0.15
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD13	11	0.15
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	2	0.15
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	2	0.15
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	2	0.15
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	2	0.15
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	2	0.15
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	2	0.15
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	2	0.15
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	2	0.15
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	16	0.15
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	16	0.15
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA2	20	0.15
(1,957)	1:32:A:LYS:HD2	1:81:A:GLY:HA3	20	0.15
(1,953)	1:8:A:VAL:HG11	1:10:A:TYR:HA	2	0.15
(1,953)	1:8:A:VAL:HG12	1:10:A:TYR:HA	2	0.15
(1,953)	1:8:A:VAL:HG13	1:10:A:TYR:HA	2	0.15
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	3	0.15
(1,945)	1:96:A:GLU:HB2	1:98:A:LEU:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:96:A:GLU:HB3	1:98:A:LEU:H	19	0.15
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	6	0.15
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	6	0.15
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	10	0.15
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	10	0.15
(1,929)	1:94:A:PRO:HA	1:96:A:GLU:H	11	0.15
(1,920)	1:94:A:PRO:HG2	1:95:A:SER:H	18	0.15
(1,920)	1:94:A:PRO:HG3	1:95:A:SER:H	18	0.15
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	14	0.15
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	20	0.15
(1,886)	1:13:A:LEU:HD21	1:92:A:ALA:H	4	0.15
(1,886)	1:13:A:LEU:HD22	1:92:A:ALA:H	4	0.15
(1,886)	1:13:A:LEU:HD23	1:92:A:ALA:H	4	0.15
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	6	0.15
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	5	0.15
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	16	0.15
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	6	0.15
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	15	0.15
(1,824)	1:84:A:HIS:HA	1:88:A:ARG:H	5	0.15
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	10	0.15
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	12	0.15
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	13	0.15
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	7	0.15
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	11	0.15
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	14	0.15
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	11	0.15
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	18	0.15
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	18	0.15
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	6	0.15
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	6	0.15
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	6	0.15
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	2	0.15
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	10	0.15
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	1	0.15
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	1	0.15
(1,772)	1:33:A:VAL:H	1:83:A:LEU:H	9	0.15
(1,767)	1:30:A:HIS:H	1:83:A:LEU:H	2	0.15
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	6	0.15
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	6	0.15
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	19	0.15
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	19	0.15
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	3	0.15
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	8	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	4	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	4	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	4	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	15	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	15	0.15
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	15	0.15
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	10	0.15
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	9	0.15
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	9	0.15
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	1	0.15
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	10	0.15
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	16	0.15
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	15	0.15
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	2	0.15
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	14	0.15
(1,680)	1:75:A:SER:HB2	1:77:A:LYS:H	17	0.15
(1,680)	1:75:A:SER:HB3	1:77:A:LYS:H	17	0.15
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	3	0.15
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	2	0.15
(1,647)	1:62:A:PHE:HB2	1:75:A:SER:H	18	0.15
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	12	0.15
(1,632)	1:63:A:GLU:HG2	1:72:A:ARG:H	16	0.15
(1,632)	1:63:A:GLU:HG3	1:72:A:ARG:H	16	0.15
(1,630)	1:39:A:PHE:HZ	1:72:A:ARG:H	6	0.15
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	15	0.15
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	16	0.15
(1,625)	1:67:A:PHE:HA	1:71:A:ALA:H	13	0.15
(1,607)	1:65:A:VAL:HG21	1:67:A:PHE:H	17	0.15
(1,607)	1:65:A:VAL:HG22	1:67:A:PHE:H	17	0.15
(1,607)	1:65:A:VAL:HG23	1:67:A:PHE:H	17	0.15
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	17	0.15
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	5	0.15
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	6	0.15
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	7	0.15
(1,563)	1:36:A:LEU:HD21	1:62:A:PHE:H	10	0.15
(1,563)	1:36:A:LEU:HD22	1:62:A:PHE:H	10	0.15
(1,563)	1:36:A:LEU:HD23	1:62:A:PHE:H	10	0.15
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	1	0.15
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	14	0.15
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	2	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	2	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	2	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	5	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	5	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	5	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	8	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	8	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	8	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	16	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	16	0.15
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	16	0.15
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	8	0.15
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	13	0.15
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	13	0.15
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB2	17	0.15
(1,530)	1:58:A:ALA:H	1:60:A:GLU:HB3	17	0.15
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	14	0.15
(1,508)	1:50:A:LEU:HA	1:54:A:ALA:H	20	0.15
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	6	0.15
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	6	0.15
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	6	0.15
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	14	0.15
(1,475)	1:48:A:GLU:HG3	1:50:A:LEU:H	6	0.15
(1,451)	1:45:A:GLY:H	1:46:A:GLY:H	6	0.15
(1,432)	1:40:A:LEU:HA	1:43:A:TRP:H	10	0.15
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	12	0.15
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	2	0.15
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	4	0.15
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	4	0.15
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	4	0.15
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	18	0.15
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	19	0.15
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	1	0.15
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	20	0.15
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	11	0.15
(1,279)	1:31:A:HIS:H	1:32:A:LYS:H	17	0.15
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	3	0.15
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	3	0.15
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	6	0.15
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	12	0.15
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	12	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	19	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	19	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	19	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	19	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	19	0.15
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	19	0.15
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	9	0.15
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	16	0.15
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	20	0.15
(1,173)	1:23:A:LYS:HG2	1:24:A:SER:H	13	0.15
(1,173)	1:23:A:LYS:HG3	1:24:A:SER:H	13	0.15
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	20	0.15
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	11	0.15
(1,156)	1:22:A:SER:H	1:23:A:LYS:HD3	16	0.15
(1,152)	1:22:A:SER:H	1:23:A:LYS:H	3	0.15
(1,152)	1:22:A:SER:H	1:23:A:LYS:H	17	0.15
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	18	0.15
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	4	0.15
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	4	0.15
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	4	0.15
(1,113)	1:12:A:THR:HG21	1:16:A:ILE:H	8	0.15
(1,113)	1:12:A:THR:HG22	1:16:A:ILE:H	8	0.15
(1,113)	1:12:A:THR:HG23	1:16:A:ILE:H	8	0.15
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	4	0.15
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	12	0.15
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	2	0.15
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	9	0.15
(1,92)	1:14:A:GLU:H	1:14:A:GLU:HB2	16	0.15
(1,92)	1:14:A:GLU:H	1:14:A:GLU:HB3	16	0.15
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	12	0.15
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	3	0.15
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	5	0.15
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	12	0.15
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	6	0.15
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	16	0.15
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	16	0.15
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	11	0.15
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	11	0.15
(1,45)	1:10:A:TYR:H	1:10:A:TYR:HE1	18	0.15
(1,45)	1:10:A:TYR:H	1:10:A:TYR:HE2	18	0.15
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	11	0.15
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	6	0.15
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	6	0.15
(1,14)	1:5:A:ASP:HB2	1:6:A:LYS:H	8	0.15
(1,14)	1:5:A:ASP:HB3	1:6:A:LYS:H	8	0.15
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	2	0.15
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	10	0.15
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	1	0.15
(3,27)	1:48:A:GLU:O	1:52:A:GLU:H	5	0.14
(3,21)	1:13:A:LEU:O	1:17:A:GLN:H	2	0.14
(3,11)	1:33:A:VAL:O	1:81:A:GLY:H	12	0.14
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	17	0.14
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG21	15	0.14
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG22	15	0.14
(2,89)	1:53:A:GLN:HE22	1:97:A:THR:HG23	15	0.14
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG21	16	0.14
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG22	16	0.14
(2,83)	1:34:A:TYR:HE1	1:80:A:ILE:HG23	16	0.14
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG21	16	0.14
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG22	16	0.14
(2,83)	1:34:A:TYR:HE2	1:80:A:ILE:HG23	16	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	12	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	12	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	12	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	18	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	18	0.14
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	18	0.14
(2,58)	1:81:A:GLY:H	1:83:A:LEU:H	7	0.14
(2,58)	1:81:A:GLY:H	1:83:A:LEU:H	9	0.14
(2,58)	1:81:A:GLY:H	1:83:A:LEU:H	13	0.14
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	2	0.14
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	14	0.14
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	12	0.14
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	12	0.14
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	12	0.14
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	14	0.14
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	14	0.14
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	14	0.14
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	19	0.14
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	19	0.14
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	19	0.14
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:19:A:HIS:HE1	1:53:A:GLN:H	19	0.14
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	14	0.14
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	16	0.14
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	12	0.14
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	12	0.14
(1,1081)	1:53:A:GLN:HE22	1:64:A:ASP:HB3	20	0.14
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	7	0.14
(1,1070)	1:39:A:PHE:HA	1:43:A:TRP:HD1	8	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	1	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	1	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	1	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	1	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	1	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	1	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	7	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	7	0.14
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	7	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	7	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	7	0.14
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	7	0.14
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	17	0.14
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	17	0.14
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	15	0.14
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	15	0.14
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	15	0.14
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	15	0.14
(1,1060)	1:39:A:PHE:HD1	1:75:A:SER:HA	16	0.14
(1,1060)	1:39:A:PHE:HD2	1:75:A:SER:HA	16	0.14
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	2	0.14
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	2	0.14
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	13	0.14
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	13	0.14
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	4	0.14
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	4	0.14
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	4	0.14
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	4	0.14
(1,1005)	1:11:A:TYR:HD1	1:81:A:GLY:HA3	16	0.14
(1,1005)	1:11:A:TYR:HD2	1:81:A:GLY:HA3	16	0.14
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	5	0.14
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	5	0.14
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	9	0.14
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	17	0.14
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	17	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	5	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	5	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	5	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	5	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	5	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	5	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	20	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	20	0.14
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	20	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	20	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	20	0.14
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	20	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	1	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	1	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	1	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	1	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	10	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	10	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	10	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	10	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	18	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	18	0.14
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	18	0.14
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	18	0.14
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	1	0.14
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	1	0.14
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	1	0.14
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	16	0.14
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	16	0.14
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	17	0.14
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	17	0.14
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	1	0.14
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	1	0.14
(1,947)	1:95:A:SER:HA	1:98:A:LEU:H	12	0.14
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	2	0.14
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	3	0.14
(1,930)	1:96:A:GLU:H	1:97:A:THR:HA	10	0.14
(1,924)	1:95:A:SER:H	1:98:A:LEU:H	1	0.14
(1,912)	1:91:A:ILE:HG12	1:93:A:LYS:H	6	0.14
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	17	0.14
(1,853)	1:87:A:ASP:HB3	1:90:A:LYS:H	11	0.14
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	11	0.14
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	17	0.14
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	18	0.14
(1,824)	1:84:A:HIS:HA	1:88:A:ARG:H	10	0.14
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	11	0.14
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	10	0.14
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	16	0.14
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	8	0.14
(1,801)	1:86:A:ASP:H	1:88:A:ARG:HE	17	0.14
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	5	0.14
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	5	0.14
(1,791)	1:12:A:THR:HG21	1:84:A:HIS:H	4	0.14
(1,791)	1:12:A:THR:HG22	1:84:A:HIS:H	4	0.14
(1,791)	1:12:A:THR:HG23	1:84:A:HIS:H	4	0.14
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	14	0.14
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	6	0.14
(1,779)	1:10:A:TYR:HA	1:84:A:HIS:H	16	0.14
(1,777)	1:10:A:TYR:HD1	1:84:A:HIS:H	3	0.14
(1,777)	1:10:A:TYR:HD2	1:84:A:HIS:H	3	0.14
(1,769)	1:32:A:LYS:HA	1:83:A:LEU:H	3	0.14
(1,762)	1:28:A:ILE:HG21	1:83:A:LEU:H	2	0.14
(1,762)	1:28:A:ILE:HG22	1:83:A:LEU:H	2	0.14
(1,762)	1:28:A:ILE:HG23	1:83:A:LEU:H	2	0.14
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	3	0.14
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	3	0.14
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	1	0.14
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	17	0.14
(1,738)	1:34:A:TYR:HA	1:81:A:GLY:H	2	0.14
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	13	0.14
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	13	0.14
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	13	0.14
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	16	0.14
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	16	0.14
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	16	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	5	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	5	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	5	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	20	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	20	0.14
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	18	0.14
(1,684)	1:77:A:LYS:H	1:78:A:TYR:HA	7	0.14
(1,680)	1:75:A:SER:HB2	1:77:A:LYS:H	15	0.14
(1,680)	1:75:A:SER:HB3	1:77:A:LYS:H	15	0.14
(1,676)	1:75:A:SER:H	1:77:A:LYS:H	7	0.14
(1,664)	1:75:A:SER:HG	1:76:A:LYS:H	9	0.14
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	4	0.14
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	10	0.14
(1,627)	1:67:A:PHE:H	1:71:A:ALA:H	5	0.14
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	5	0.14
(1,620)	1:69:A:THR:HG21	1:71:A:ALA:H	14	0.14
(1,620)	1:69:A:THR:HG22	1:71:A:ALA:H	14	0.14
(1,620)	1:69:A:THR:HG23	1:71:A:ALA:H	14	0.14
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	19	0.14
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	4	0.14
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	2	0.14
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	4	0.14
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	19	0.14
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	13	0.14
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	13	0.14
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	15	0.14
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	5	0.14
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	11	0.14
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	11	0.14
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	12	0.14
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	12	0.14
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	4	0.14
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	4	0.14
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	4	0.14
(1,514)	1:55:A:GLY:HA3	1:56:A:GLY:H	2	0.14
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	18	0.14
(1,453)	1:46:A:GLY:H	1:47:A:GLU:HA	9	0.14
(1,432)	1:40:A:LEU:HA	1:43:A:TRP:H	11	0.14
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	6	0.14
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	6	0.14
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	11	0.14
(1,420)	1:39:A:PHE:HD1	1:42:A:GLU:H	7	0.14
(1,420)	1:39:A:PHE:HD2	1:42:A:GLU:H	7	0.14
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	16	0.14
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	16	0.14
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	16	0.14
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	5	0.14
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	5	0.14
(1,411)	1:40:A:LEU:HD21	1:41:A:GLU:H	15	0.14
(1,411)	1:40:A:LEU:HD22	1:41:A:GLU:H	15	0.14
(1,411)	1:40:A:LEU:HD23	1:41:A:GLU:H	15	0.14
(1,396)	1:39:A:PHE:HD1	1:40:A:LEU:H	4	0.14
(1,396)	1:39:A:PHE:HD2	1:40:A:LEU:H	4	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	2	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	2	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	2	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	3	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	3	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	3	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	9	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	9	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	9	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	17	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	17	0.14
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	17	0.14
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	3	0.14
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	3	0.14
(1,369)	1:36:A:LEU:HG	1:37:A:THR:H	4	0.14
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	10	0.14
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	17	0.14
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	18	0.14
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	5	0.14
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	5	0.14
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	5	0.14
(1,326)	1:35:A:ASP:H	1:79:A:ILE:H	12	0.14
(1,322)	1:34:A:TYR:HB3	1:35:A:ASP:H	18	0.14
(1,302)	1:28:A:ILE:HA	1:34:A:TYR:H	8	0.14
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	1	0.14
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	3	0.14
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	18	0.14
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	5	0.14
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	17	0.14
(1,280)	1:31:A:HIS:HB2	1:32:A:LYS:H	1	0.14
(1,280)	1:31:A:HIS:HB2	1:32:A:LYS:H	19	0.14
(1,276)	1:30:A:HIS:HD1	1:32:A:LYS:H	14	0.14
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	14	0.14
(1,272)	1:31:A:HIS:H	1:31:A:HIS:HB3	19	0.14
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	16	0.14
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	8	0.14
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	15	0.14
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	16	0.14
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	5	0.14
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	5	0.14
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	1	0.14
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	13	0.14
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	9	0.14
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	18	0.14
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	15	0.14
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	15	0.14
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	15	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	2	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	2	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	2	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	2	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	2	0.14
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	2	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	1	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	1	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	1	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	11	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	11	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	11	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	17	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	17	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	17	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	20	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	20	0.14
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	20	0.14
(1,209)	1:26:A:TRP:HA	1:27:A:VAL:H	10	0.14
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	5	0.14
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	2	0.14
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	7	0.14
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	17	0.14
(1,197)	1:25:A:THR:HG21	1:26:A:TRP:H	19	0.14
(1,197)	1:25:A:THR:HG22	1:26:A:TRP:H	19	0.14
(1,197)	1:25:A:THR:HG23	1:26:A:TRP:H	19	0.14
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	4	0.14
(1,191)	1:25:A:THR:H	1:37:A:THR:H	3	0.14
(1,180)	1:23:A:LYS:HE2	1:24:A:SER:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:23:A:LYS:HE3	1:24:A:SER:H	19	0.14
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	9	0.14
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	17	0.14
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	13	0.14
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG2	3	0.14
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG3	3	0.14
(1,158)	1:22:A:SER:H	1:24:A:SER:H	3	0.14
(1,138)	1:20:A:LYS:HB2	1:21:A:ASP:H	18	0.14
(1,138)	1:20:A:LYS:HB3	1:21:A:ASP:H	18	0.14
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	16	0.14
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	3	0.14
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	3	0.14
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	3	0.14
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	16	0.14
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	6	0.14
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	1	0.14
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	13	0.14
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	18	0.14
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	7	0.14
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	7	0.14
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG12	10	0.14
(1,70)	1:12:A:THR:H	1:16:A:ILE:HG13	10	0.14
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	15	0.14
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	15	0.14
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	6	0.14
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	6	0.14
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	16	0.14
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	16	0.14
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	11	0.14
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	11	0.14
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	18	0.14
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	18	0.14
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	12	0.14
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD2	13	0.14
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD3	13	0.14
(1,7)	1:4:A:SER:HB2	1:5:A:ASP:H	15	0.14
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	14	0.14
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	16	0.14
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	20	0.14
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	6	0.14
(3,33)	1:70:A:ASP:O	1:74:A:LEU:H	6	0.13
(3,22)	1:38:A:LYS:O	1:42:A:GLU:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	10	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	8	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	8	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	8	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG21	11	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG22	11	0.13
(2,78)	1:26:A:TRP:HE3	1:80:A:ILE:HG23	11	0.13
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE1	15	0.13
(2,73)	1:8:A:VAL:HG21	1:11:A:TYR:HE2	15	0.13
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE1	15	0.13
(2,73)	1:8:A:VAL:HG22	1:11:A:TYR:HE2	15	0.13
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE1	15	0.13
(2,73)	1:8:A:VAL:HG23	1:11:A:TYR:HE2	15	0.13
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	11	0.13
(2,64)	1:89:A:SER:HG	1:91:A:ILE:H	4	0.13
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	15	0.13
(2,38)	1:67:A:PHE:H	1:68:A:SER:HG	9	0.13
(2,34)	1:53:A:GLN:HE22	1:57:A:ASP:H	13	0.13
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	2	0.13
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	2	0.13
(2,18)	1:16:A:ILE:HG12	1:27:A:VAL:H	1	0.13
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	17	0.13
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	13	0.13
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	17	0.13
(1,1108)	1:12:A:THR:HG21	1:83:A:LEU:HA	5	0.13
(1,1108)	1:12:A:THR:HG22	1:83:A:LEU:HA	5	0.13
(1,1108)	1:12:A:THR:HG23	1:83:A:LEU:HA	5	0.13
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD1	18	0.13
(1,1099)	1:66:A:GLY:HA2	1:67:A:PHE:HD2	18	0.13
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD1	18	0.13
(1,1099)	1:66:A:GLY:HA3	1:67:A:PHE:HD2	18	0.13
(1,1079)	1:53:A:GLN:HB2	1:53:A:GLN:HE22	9	0.13
(1,1079)	1:53:A:GLN:HB3	1:53:A:GLN:HE22	9	0.13
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB1	2	0.13
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB2	2	0.13
(1,1066)	1:39:A:PHE:HE1	1:71:A:ALA:HB3	2	0.13
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB1	2	0.13
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB2	2	0.13
(1,1066)	1:39:A:PHE:HE2	1:71:A:ALA:HB3	2	0.13
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	10	0.13
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	10	0.13
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	2	0.13
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	2	0.13
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	2	0.13
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	2	0.13
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	2	0.13
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	2	0.13
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	14	0.13
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	14	0.13
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	14	0.13
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	14	0.13
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	14	0.13
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	14	0.13
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	14	0.13
(1,1027)	1:11:A:TYR:HD1	1:26:A:TRP:HB2	15	0.13
(1,1027)	1:11:A:TYR:HD2	1:26:A:TRP:HB2	15	0.13
(1,1022)	1:25:A:THR:HG21	1:26:A:TRP:HE3	2	0.13
(1,1022)	1:25:A:THR:HG22	1:26:A:TRP:HE3	2	0.13
(1,1022)	1:25:A:THR:HG23	1:26:A:TRP:HE3	2	0.13
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	8	0.13
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	8	0.13
(1,1014)	1:11:A:TYR:HD1	1:26:A:TRP:HE3	9	0.13
(1,1014)	1:11:A:TYR:HD2	1:26:A:TRP:HE3	9	0.13
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	8	0.13
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	8	0.13
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG21	19	0.13
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG22	19	0.13
(1,997)	1:11:A:TYR:HD1	1:12:A:THR:HG23	19	0.13
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG21	19	0.13
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG22	19	0.13
(1,997)	1:11:A:TYR:HD2	1:12:A:THR:HG23	19	0.13
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	13	0.13
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	13	0.13
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	13	0.13
(1,977)	1:11:A:TYR:HE1	1:80:A:ILE:HB	7	0.13
(1,977)	1:11:A:TYR:HE2	1:80:A:ILE:HB	7	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	2	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	2	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	4	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	4	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	15	0.13
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	15	0.13
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	20	0.13
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	20	0.13
(1,949)	1:94:A:PRO:HA	1:98:A:LEU:H	16	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	1	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	4	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	7	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	12	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	14	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	16	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	19	0.13
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	20	0.13
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	1	0.13
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	1	0.13
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	2	0.13
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	2	0.13
(1,935)	1:96:A:GLU:HG2	1:97:A:THR:H	9	0.13
(1,935)	1:96:A:GLU:HG3	1:97:A:THR:H	9	0.13
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB2	3	0.13
(1,926)	1:96:A:GLU:H	1:96:A:GLU:HB3	3	0.13
(1,917)	1:94:A:PRO:HA	1:95:A:SER:H	15	0.13
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	20	0.13
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	7	0.13
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	9	0.13
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	7	0.13
(1,855)	1:88:A:ARG:H	1:90:A:LYS:H	8	0.13
(1,855)	1:88:A:ARG:H	1:90:A:LYS:H	20	0.13
(1,849)	1:87:A:ASP:HB2	1:90:A:LYS:H	3	0.13
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	4	0.13
(1,848)	1:86:A:ASP:HA	1:90:A:LYS:H	11	0.13
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	5	0.13
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	1	0.13
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	4	0.13
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	7	0.13
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	1	0.13
(1,805)	1:87:A:ASP:H	1:88:A:ARG:HA	20	0.13
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	6	0.13
(1,804)	1:12:A:THR:HB	1:87:A:ASP:H	15	0.13
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	18	0.13
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	7	0.13
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	7	0.13
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	18	0.13
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	18	0.13
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	14	0.13
(1,727)	1:78:A:TYR:HA	1:80:A:ILE:H	5	0.13
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	11	0.13
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	11	0.13
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	11	0.13
(1,719)	1:34:A:TYR:HB3	1:80:A:ILE:H	6	0.13
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	13	0.13
(1,718)	1:79:A:ILE:HB	1:80:A:ILE:H	16	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	1	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	1	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	1	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	5	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	5	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	5	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	18	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	18	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	18	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	20	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	20	0.13
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	20	0.13
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	3	0.13
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	15	0.13
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	5	0.13
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	7	0.13
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD1	12	0.13
(1,695)	1:78:A:TYR:H	1:78:A:TYR:HD2	12	0.13
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	11	0.13
(1,688)	1:35:A:ASP:H	1:78:A:TYR:H	4	0.13
(1,680)	1:75:A:SER:HB2	1:77:A:LYS:H	12	0.13
(1,680)	1:75:A:SER:HB3	1:77:A:LYS:H	12	0.13
(1,663)	1:73:A:GLU:HA	1:76:A:LYS:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:62:A:PHE:HD1	1:76:A:LYS:H	17	0.13
(1,662)	1:62:A:PHE:HD2	1:76:A:LYS:H	17	0.13
(1,657)	1:75:A:SER:H	1:76:A:LYS:HB2	10	0.13
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	10	0.13
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	19	0.13
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	6	0.13
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE1	20	0.13
(1,608)	1:67:A:PHE:H	1:67:A:PHE:HE2	20	0.13
(1,600)	1:63:A:GLU:HA	1:66:A:GLY:H	18	0.13
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	12	0.13
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	15	0.13
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	18	0.13
(1,577)	1:61:A:ASN:HA	1:64:A:ASP:H	18	0.13
(1,576)	1:61:A:ASN:HD22	1:64:A:ASP:H	4	0.13
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	18	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	1	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	1	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	1	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	14	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	14	0.13
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	14	0.13
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	5	0.13
(1,515)	1:56:A:GLY:H	1:56:A:GLY:HA3	2	0.13
(1,510)	1:54:A:ALA:H	1:55:A:GLY:HA3	6	0.13
(1,510)	1:54:A:ALA:H	1:55:A:GLY:HA3	7	0.13
(1,503)	1:53:A:GLN:H	1:54:A:ALA:HA	9	0.13
(1,494)	1:49:A:VAL:HA	1:52:A:GLU:H	2	0.13
(1,491)	1:49:A:VAL:HG21	1:52:A:GLU:H	1	0.13
(1,491)	1:49:A:VAL:HG22	1:52:A:GLU:H	1	0.13
(1,491)	1:49:A:VAL:HG23	1:52:A:GLU:H	1	0.13
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	1	0.13
(1,484)	1:48:A:GLU:H	1:51:A:ARG:H	12	0.13
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	8	0.13
(1,454)	1:46:A:GLY:H	1:47:A:GLU:H	6	0.13
(1,451)	1:45:A:GLY:H	1:46:A:GLY:H	17	0.13
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	2	0.13
(1,435)	1:42:A:GLU:H	1:43:A:TRP:H	19	0.13
(1,432)	1:40:A:LEU:HA	1:43:A:TRP:H	16	0.13
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB2	2	0.13
(1,430)	1:42:A:GLU:H	1:43:A:TRP:HB3	2	0.13
(1,423)	1:40:A:LEU:HA	1:42:A:GLU:H	19	0.13
(1,412)	1:36:A:LEU:HD11	1:41:A:GLU:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:36:A:LEU:HD12	1:41:A:GLU:H	2	0.13
(1,412)	1:36:A:LEU:HD13	1:41:A:GLU:H	2	0.13
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	15	0.13
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	16	0.13
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	16	0.13
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	16	0.13
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	16	0.13
(1,391)	1:36:A:LEU:HD21	1:40:A:LEU:H	12	0.13
(1,391)	1:36:A:LEU:HD22	1:40:A:LEU:H	12	0.13
(1,391)	1:36:A:LEU:HD23	1:40:A:LEU:H	12	0.13
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	7	0.13
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	7	0.13
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	20	0.13
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	3	0.13
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	5	0.13
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	18	0.13
(1,344)	1:26:A:TRP:HB2	1:36:A:LEU:H	19	0.13
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	11	0.13
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	4	0.13
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	4	0.13
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	4	0.13
(1,318)	1:33:A:VAL:HG21	1:34:A:TYR:H	14	0.13
(1,318)	1:33:A:VAL:HG22	1:34:A:TYR:H	14	0.13
(1,318)	1:33:A:VAL:HG23	1:34:A:TYR:H	14	0.13
(1,318)	1:33:A:VAL:HG21	1:34:A:TYR:H	18	0.13
(1,318)	1:33:A:VAL:HG22	1:34:A:TYR:H	18	0.13
(1,318)	1:33:A:VAL:HG23	1:34:A:TYR:H	18	0.13
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	12	0.13
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	12	0.13
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	4	0.13
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	4	0.13
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	4	0.13
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	15	0.13
(1,263)	1:30:A:HIS:HE1	1:31:A:HIS:H	20	0.13
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	9	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	7	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	7	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	12	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	12	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE1	19	0.13
(1,253)	1:30:A:HIS:H	1:34:A:TYR:HE2	19	0.13
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	4	0.13
(1,236)	1:28:A:ILE:H	1:58:A:ALA:HA	11	0.13
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	20	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	4	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	4	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	4	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	6	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	6	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	6	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	7	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	7	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	7	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	16	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	16	0.13
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	16	0.13
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	1	0.13
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	7	0.13
(1,191)	1:25:A:THR:H	1:37:A:THR:H	19	0.13
(1,177)	1:19:A:HIS:HB2	1:24:A:SER:H	1	0.13
(1,177)	1:19:A:HIS:HB3	1:24:A:SER:H	1	0.13
(1,176)	1:19:A:HIS:HA	1:24:A:SER:H	4	0.13
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	9	0.13
(1,169)	1:23:A:LYS:H	1:24:A:SER:H	19	0.13
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	3	0.13
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	3	0.13
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	4	0.13
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	4	0.13
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	4	0.13
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD2	9	0.13
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD3	9	0.13
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	20	0.13
(1,137)	1:20:A:LYS:HD2	1:21:A:ASP:H	20	0.13
(1,137)	1:20:A:LYS:HD3	1:21:A:ASP:H	20	0.13
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	6	0.13
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	17	0.13
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	4	0.13
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	11	0.13
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	6	0.13
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	8	0.13
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	17	0.13
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	19	0.13
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	3	0.13
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	13	0.13
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	13	0.13
(1,58)	1:11:A:TYR:HD1	1:12:A:THR:H	10	0.13
(1,58)	1:11:A:TYR:HD2	1:12:A:THR:H	10	0.13
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	12	0.13
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	12	0.13
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	7	0.13
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	14	0.13
(1,12)	1:4:A:SER:H	1:6:A:LYS:H	19	0.13
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	3	0.13
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	9	0.13
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	11	0.13
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	17	0.13
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	19	0.13
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	7	0.13
(1,3)	1:4:A:SER:H	1:4:A:SER:HG	8	0.13
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	14	0.13
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	18	0.13
(3,34)	1:70:A:ASP:O	1:74:A:LEU:N	9	0.12
(3,28)	1:48:A:GLU:O	1:52:A:GLU:N	9	0.12
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	15	0.12
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	3	0.12
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	14	0.12
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE1	18	0.12
(2,72)	1:5:A:ASP:HB3	1:11:A:TYR:HE2	18	0.12
(2,66)	1:90:A:LYS:HA	1:93:A:LYS:H	1	0.12
(2,61)	1:31:A:HIS:HD2	1:87:A:ASP:H	12	0.12
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	16	0.12
(2,51)	1:33:A:VAL:HB	1:80:A:ILE:H	17	0.12
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	9	0.12
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	5	0.12
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	2	0.12
(2,5)	1:14:A:GLU:H	1:84:A:HIS:HD1	15	0.12
(2,3)	1:11:A:TYR:H	1:84:A:HIS:HB2	15	0.12
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE1	6	0.12
(1,1104)	1:75:A:SER:HA	1:78:A:TYR:HE2	6	0.12
(1,1094)	1:62:A:PHE:HD1	1:75:A:SER:HG	19	0.12
(1,1094)	1:62:A:PHE:HD2	1:75:A:SER:HG	19	0.12
(1,1090)	1:61:A:ASN:HD21	1:64:A:ASP:H	6	0.12
(1,1078)	1:52:A:GLU:HG3	1:53:A:GLN:HE22	17	0.12
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:39:A:PHE:HE1	1:62:A:PHE:HB3	18	0.12
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB2	18	0.12
(1,1063)	1:39:A:PHE:HE2	1:62:A:PHE:HB3	18	0.12
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	6	0.12
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	6	0.12
(1,1051)	1:34:A:TYR:HD1	1:78:A:TYR:HA	10	0.12
(1,1051)	1:34:A:TYR:HD2	1:78:A:TYR:HA	10	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	1	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	1	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	13	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	13	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	15	0.12
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	15	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	15	0.12
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	15	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	15	0.12
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	15	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	15	0.12
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	15	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	15	0.12
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	15	0.12
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	15	0.12
(1,1016)	1:16:A:ILE:HA	1:26:A:TRP:HE3	18	0.12
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD11	10	0.12
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD12	10	0.12
(1,998)	1:11:A:TYR:HD1	1:16:A:ILE:HD13	10	0.12
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD11	10	0.12
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD12	10	0.12
(1,998)	1:11:A:TYR:HD2	1:16:A:ILE:HD13	10	0.12
(1,992)	1:11:A:TYR:HA	1:83:A:LEU:HA	19	0.12
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	2	0.12
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	2	0.12
(1,982)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	19	0.12
(1,982)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	19	0.12
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	2	0.12
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	2	0.12
(1,979)	1:11:A:TYR:HE1	1:26:A:TRP:HD1	19	0.12
(1,979)	1:11:A:TYR:HE2	1:26:A:TRP:HD1	19	0.12
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	12	0.12
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	12	0.12
(1,917)	1:94:A:PRO:HA	1:95:A:SER:H	13	0.12
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	10	0.12
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	10	0.12
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	5	0.12
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	14	0.12
(1,887)	1:87:A:ASP:HA	1:92:A:ALA:H	6	0.12
(1,879)	1:91:A:ILE:H	1:92:A:ALA:HB1	5	0.12
(1,879)	1:91:A:ILE:H	1:92:A:ALA:HB2	5	0.12
(1,879)	1:91:A:ILE:H	1:92:A:ALA:HB3	5	0.12
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	12	0.12
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	9	0.12
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	20	0.12
(1,822)	1:85:A:PRO:HA	1:88:A:ARG:H	1	0.12
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	17	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	6	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	9	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	10	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	14	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	15	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	17	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	18	0.12
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	20	0.12
(1,807)	1:84:A:HIS:HA	1:87:A:ASP:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	9	0.12
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	3	0.12
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	16	0.12
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	16	0.12
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	16	0.12
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	8	0.12
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	8	0.12
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	11	0.12
(1,721)	1:33:A:VAL:HG21	1:80:A:ILE:H	6	0.12
(1,721)	1:33:A:VAL:HG22	1:80:A:ILE:H	6	0.12
(1,721)	1:33:A:VAL:HG23	1:80:A:ILE:H	6	0.12
(1,721)	1:33:A:VAL:HG21	1:80:A:ILE:H	10	0.12
(1,721)	1:33:A:VAL:HG22	1:80:A:ILE:H	10	0.12
(1,721)	1:33:A:VAL:HG23	1:80:A:ILE:H	10	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	8	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	8	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	8	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	11	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	11	0.12
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	11	0.12
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	10	0.12
(1,708)	1:78:A:TYR:HA	1:79:A:ILE:H	15	0.12
(1,700)	1:34:A:TYR:HD1	1:78:A:TYR:H	7	0.12
(1,700)	1:34:A:TYR:HD2	1:78:A:TYR:H	7	0.12
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	8	0.12
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	10	0.12
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	14	0.12
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	10	0.12
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	10	0.12
(1,655)	1:75:A:SER:H	1:75:A:SER:HB2	1	0.12
(1,655)	1:75:A:SER:H	1:75:A:SER:HB3	1	0.12
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	18	0.12
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG2	14	0.12
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG3	14	0.12
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG2	16	0.12
(1,642)	1:72:A:ARG:H	1:73:A:GLU:HG3	16	0.12
(1,630)	1:39:A:PHE:HZ	1:72:A:ARG:H	19	0.12
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	3	0.12
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	18	0.12
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD1	7	0.12
(1,611)	1:67:A:PHE:H	1:67:A:PHE:HD2	7	0.12
(1,593)	1:61:A:ASN:HA	1:66:A:GLY:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:61:A:ASN:HD21	1:64:A:ASP:H	1	0.12
(1,577)	1:61:A:ASN:HA	1:64:A:ASP:H	9	0.12
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	4	0.12
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	9	0.12
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB3	5	0.12
(1,559)	1:61:A:ASN:H	1:62:A:PHE:HB2	5	0.12
(1,557)	1:29:A:LEU:HA	1:61:A:ASN:H	10	0.12
(1,553)	1:60:A:GLU:HA	1:61:A:ASN:H	2	0.12
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	3	0.12
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	14	0.12
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	12	0.12
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	12	0.12
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	12	0.12
(1,542)	1:58:A:ALA:HB1	1:59:A:THR:H	7	0.12
(1,542)	1:58:A:ALA:HB2	1:59:A:THR:H	7	0.12
(1,542)	1:58:A:ALA:HB3	1:59:A:THR:H	7	0.12
(1,539)	1:29:A:LEU:H	1:59:A:THR:H	16	0.12
(1,520)	1:56:A:GLY:HA3	1:57:A:ASP:H	3	0.12
(1,481)	1:50:A:LEU:H	1:52:A:GLU:H	16	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	10	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	10	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	10	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	14	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	14	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	14	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	15	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	15	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	15	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	19	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	19	0.12
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	19	0.12
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	1	0.12
(1,451)	1:45:A:GLY:H	1:46:A:GLY:H	7	0.12
(1,449)	1:40:A:LEU:HB2	1:46:A:GLY:H	20	0.12
(1,449)	1:40:A:LEU:HB3	1:46:A:GLY:H	20	0.12
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD21	6	0.12
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD22	6	0.12
(1,448)	1:46:A:GLY:H	1:50:A:LEU:HD23	6	0.12
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	18	0.12
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	18	0.12
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	18	0.12
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	18	0.12
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	18	0.12
(1,431)	1:39:A:PHE:HA	1:43:A:TRP:H	18	0.12
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	4	0.12
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	7	0.12
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	9	0.12
(1,398)	1:39:A:PHE:H	1:40:A:LEU:H	19	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	10	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	10	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	17	0.12
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	17	0.12
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	9	0.12
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	12	0.12
(1,376)	1:36:A:LEU:HA	1:38:A:LYS:H	13	0.12
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	13	0.12
(1,358)	1:27:A:VAL:H	1:37:A:THR:H	17	0.12
(1,340)	1:35:A:ASP:H	1:79:A:ILE:HA	1	0.12
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	4	0.12
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	4	0.12
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	4	0.12
(1,336)	1:35:A:ASP:H	1:80:A:ILE:H	6	0.12
(1,331)	1:35:A:ASP:H	1:78:A:TYR:HA	14	0.12
(1,321)	1:34:A:TYR:H	1:83:A:LEU:HB2	19	0.12
(1,314)	1:29:A:LEU:HD21	1:34:A:TYR:H	3	0.12
(1,314)	1:29:A:LEU:HD22	1:34:A:TYR:H	3	0.12
(1,314)	1:29:A:LEU:HD23	1:34:A:TYR:H	3	0.12
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	10	0.12
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	14	0.12
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	8	0.12
(1,301)	1:33:A:VAL:H	1:81:A:GLY:HA3	16	0.12
(1,280)	1:31:A:HIS:HB2	1:32:A:LYS:H	3	0.12
(1,272)	1:31:A:HIS:H	1:31:A:HIS:HB3	9	0.12
(1,270)	1:31:A:HIS:H	1:31:A:HIS:HB2	4	0.12
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE1	14	0.12
(1,265)	1:31:A:HIS:H	1:34:A:TYR:HE2	14	0.12
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	10	0.12
(1,246)	1:29:A:LEU:H	1:29:A:LEU:HG	11	0.12
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	2	0.12
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	9	0.12
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD21	15	0.12
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD22	15	0.12
(1,222)	1:28:A:ILE:H	1:36:A:LEU:HD23	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	7	0.12
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	7	0.12
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	7	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	9	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	9	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	9	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	12	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	12	0.12
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	12	0.12
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	8	0.12
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	11	0.12
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	12	0.12
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	14	0.12
(1,195)	1:25:A:THR:HB	1:26:A:TRP:H	18	0.12
(1,191)	1:25:A:THR:H	1:37:A:THR:H	15	0.12
(1,172)	1:23:A:LYS:H	1:37:A:THR:HA	1	0.12
(1,158)	1:22:A:SER:H	1:24:A:SER:H	10	0.12
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB2	11	0.12
(1,155)	1:22:A:SER:H	1:23:A:LYS:HB3	11	0.12
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	15	0.12
(1,147)	1:21:A:ASP:H	1:24:A:SER:H	16	0.12
(1,144)	1:21:A:ASP:H	1:24:A:SER:HB2	6	0.12
(1,144)	1:21:A:ASP:H	1:24:A:SER:HB3	6	0.12
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG2	13	0.12
(1,129)	1:19:A:HIS:H	1:51:A:ARG:HG3	13	0.12
(1,123)	1:18:A:LYS:HA	1:19:A:HIS:H	2	0.12
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	19	0.12
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	16	0.12
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	10	0.12
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	11	0.12
(1,110)	1:15:A:GLU:H	1:17:A:GLN:H	17	0.12
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	16	0.12
(1,83)	1:13:A:LEU:H	1:87:A:ASP:HB2	17	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	2	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	4	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	7	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	10	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	14	0.12
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	15	0.12
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	15	0.12
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	8	0.12
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:11:A:TYR:HE1	1:12:A:THR:H	19	0.12
(1,59)	1:11:A:TYR:HE2	1:12:A:THR:H	19	0.12
(1,33)	1:9:A:LYS:H	1:11:A:TYR:HE1	9	0.12
(1,33)	1:9:A:LYS:H	1:11:A:TYR:HE2	9	0.12
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG2	3	0.12
(1,29)	1:9:A:LYS:H	1:82:A:GLU:HG3	3	0.12
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	7	0.12
(1,4)	1:4:A:SER:H	1:4:A:SER:HB2	18	0.12
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	2	0.12
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	4	0.12
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	9	0.12
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	11	0.12
(1,1)	1:3:A:GLN:H	1:4:A:SER:H	20	0.12
(3,24)	1:37:A:THR:O	1:41:A:GLU:H	6	0.11
(3,24)	1:37:A:THR:O	1:41:A:GLU:H	17	0.11
(3,19)	1:26:A:TRP:O	1:55:A:GLY:H	7	0.11
(3,15)	1:9:A:LYS:O	1:82:A:GLU:H	5	0.11
(3,12)	1:33:A:VAL:O	1:81:A:GLY:N	12	0.11
(3,9)	1:29:A:LEU:H	1:32:A:LYS:O	15	0.11
(2,67)	1:95:A:SER:H	1:97:A:THR:HA	5	0.11
(2,56)	1:79:A:ILE:H	1:81:A:GLY:H	19	0.11
(2,45)	1:71:A:ALA:HB1	1:76:A:LYS:H	3	0.11
(2,45)	1:71:A:ALA:HB2	1:76:A:LYS:H	3	0.11
(2,45)	1:71:A:ALA:HB3	1:76:A:LYS:H	3	0.11
(2,44)	1:71:A:ALA:HA	1:76:A:LYS:H	19	0.11
(2,42)	1:69:A:THR:HG1	1:72:A:ARG:H	6	0.11
(2,30)	1:51:A:ARG:H	1:54:A:ALA:HA	17	0.11
(2,28)	1:40:A:LEU:HD21	1:49:A:VAL:H	3	0.11
(2,28)	1:40:A:LEU:HD22	1:49:A:VAL:H	3	0.11
(2,28)	1:40:A:LEU:HD23	1:49:A:VAL:H	3	0.11
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE1	12	0.11
(2,26)	1:40:A:LEU:H	1:78:A:TYR:HE2	12	0.11
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD1	6	0.11
(2,23)	1:36:A:LEU:H	1:39:A:PHE:HD2	6	0.11
(2,13)	1:16:A:ILE:H	1:19:A:HIS:H	5	0.11
(2,2)	1:10:A:TYR:H	1:84:A:HIS:HD2	13	0.11
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD2	1	0.11
(1,1110)	1:84:A:HIS:HD2	1:85:A:PRO:HD3	1	0.11
(1,1075)	1:43:A:TRP:HA	1:43:A:TRP:HD1	3	0.11
(1,1064)	1:39:A:PHE:HE1	1:67:A:PHE:HB3	1	0.11
(1,1064)	1:39:A:PHE:HE2	1:67:A:PHE:HB3	1	0.11
(1,1060)	1:39:A:PHE:HD1	1:75:A:SER:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:39:A:PHE:HD2	1:75:A:SER:HA	19	0.11
(1,1050)	1:34:A:TYR:HD1	1:76:A:LYS:HA	18	0.11
(1,1050)	1:34:A:TYR:HD2	1:76:A:LYS:HA	18	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	6	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	6	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	10	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	10	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	18	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	18	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	19	0.11
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	19	0.11
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	19	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	19	0.11
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	19	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	19	0.11
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	19	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	19	0.11
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	19	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	19	0.11
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	19	0.11
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	2	0.11
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	2	0.11
(1,1043)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	2	0.11
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	2	0.11
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	2	0.11
(1,1043)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	2	0.11
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG21	2	0.11
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG22	2	0.11
(1,1037)	1:34:A:TYR:HD1	1:80:A:ILE:HG23	2	0.11
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG21	2	0.11
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG22	2	0.11
(1,1037)	1:34:A:TYR:HD2	1:80:A:ILE:HG23	2	0.11
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD1	3	0.11
(1,1029)	1:26:A:TRP:HB3	1:34:A:TYR:HD2	3	0.11
(1,1022)	1:25:A:THR:HG21	1:26:A:TRP:HE3	14	0.11
(1,1022)	1:25:A:THR:HG22	1:26:A:TRP:HE3	14	0.11
(1,1022)	1:25:A:THR:HG23	1:26:A:TRP:HE3	14	0.11
(1,1020)	1:25:A:THR:HA	1:26:A:TRP:HE3	2	0.11
(1,1018)	1:16:A:ILE:HD11	1:26:A:TRP:HE3	8	0.11
(1,1018)	1:16:A:ILE:HD12	1:26:A:TRP:HE3	8	0.11
(1,1018)	1:16:A:ILE:HD13	1:26:A:TRP:HE3	8	0.11
(1,1018)	1:16:A:ILE:HD11	1:26:A:TRP:HE3	18	0.11
(1,1018)	1:16:A:ILE:HD12	1:26:A:TRP:HE3	18	0.11
(1,1018)	1:16:A:ILE:HD13	1:26:A:TRP:HE3	18	0.11
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG12	10	0.11
(1,1010)	1:26:A:TRP:HD1	1:80:A:ILE:HG13	10	0.11
(1,1004)	1:11:A:TYR:HD1	1:12:A:THR:HA	17	0.11
(1,1004)	1:11:A:TYR:HD2	1:12:A:THR:HA	17	0.11
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	3	0.11
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	3	0.11
(1,1000)	1:11:A:TYR:HD1	1:26:A:TRP:HD1	4	0.11
(1,1000)	1:11:A:TYR:HD2	1:26:A:TRP:HD1	4	0.11
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	13	0.11
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	13	0.11
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	18	0.11
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	18	0.11
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	18	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	6	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	6	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	11	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	11	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	20	0.11
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	20	0.11
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB2	9	0.11
(1,950)	1:98:A:LEU:H	1:98:A:LEU:HB3	9	0.11
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	6	0.11
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	9	0.11
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	11	0.11
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG2	6	0.11
(1,906)	1:93:A:LYS:H	1:94:A:PRO:HG3	6	0.11
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	10	0.11
(1,904)	1:91:A:ILE:HA	1:93:A:LYS:H	12	0.11
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	19	0.11
(1,898)	1:89:A:SER:HA	1:92:A:ALA:H	20	0.11
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	8	0.11
(1,894)	1:91:A:ILE:HA	1:92:A:ALA:H	19	0.11
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	2	0.11
(1,882)	1:91:A:ILE:H	1:92:A:ALA:HA	18	0.11
(1,866)	1:90:A:LYS:H	1:92:A:ALA:HA	13	0.11
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	2	0.11
(1,824)	1:84:A:HIS:HA	1:88:A:ARG:H	20	0.11
(1,821)	1:87:A:ASP:HB3	1:88:A:ARG:H	9	0.11
(1,820)	1:87:A:ASP:H	1:88:A:ARG:HB3	18	0.11
(1,816)	1:87:A:ASP:H	1:87:A:ASP:HB3	20	0.11
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	3	0.11
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	11	0.11
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	19	0.11
(1,806)	1:83:A:LEU:HD11	1:87:A:ASP:H	7	0.11
(1,806)	1:83:A:LEU:HD12	1:87:A:ASP:H	7	0.11
(1,806)	1:83:A:LEU:HD13	1:87:A:ASP:H	7	0.11
(1,806)	1:83:A:LEU:HD21	1:87:A:ASP:H	7	0.11
(1,806)	1:83:A:LEU:HD22	1:87:A:ASP:H	7	0.11
(1,806)	1:83:A:LEU:HD23	1:87:A:ASP:H	7	0.11
(1,802)	1:85:A:PRO:HA	1:87:A:ASP:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	13	0.11
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	13	0.11
(1,784)	1:13:A:LEU:H	1:84:A:HIS:H	14	0.11
(1,782)	1:11:A:TYR:HB2	1:84:A:HIS:H	19	0.11
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	17	0.11
(1,761)	1:11:A:TYR:HD1	1:83:A:LEU:H	20	0.11
(1,761)	1:11:A:TYR:HD2	1:83:A:LEU:H	20	0.11
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	20	0.11
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	20	0.11
(1,739)	1:79:A:ILE:HB	1:81:A:GLY:H	20	0.11
(1,737)	1:33:A:VAL:HG21	1:81:A:GLY:H	4	0.11
(1,737)	1:33:A:VAL:HG22	1:81:A:GLY:H	4	0.11
(1,737)	1:33:A:VAL:HG23	1:81:A:GLY:H	4	0.11
(1,735)	1:35:A:ASP:H	1:81:A:GLY:H	20	0.11
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	17	0.11
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	17	0.11
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	17	0.11
(1,716)	1:79:A:ILE:H	1:80:A:ILE:H	6	0.11
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	19	0.11
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	19	0.11
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	19	0.11
(1,709)	1:79:A:ILE:H	1:80:A:ILE:HA	16	0.11
(1,693)	1:77:A:LYS:H	1:78:A:TYR:H	6	0.11
(1,692)	1:77:A:LYS:HD2	1:78:A:TYR:H	12	0.11
(1,692)	1:77:A:LYS:HD3	1:78:A:TYR:H	12	0.11
(1,686)	1:76:A:LYS:HE2	1:77:A:LYS:H	1	0.11
(1,686)	1:76:A:LYS:HE3	1:77:A:LYS:H	1	0.11
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE1	18	0.11
(1,675)	1:77:A:LYS:H	1:78:A:TYR:HE2	18	0.11
(1,660)	1:75:A:SER:H	1:78:A:TYR:H	3	0.11
(1,655)	1:75:A:SER:H	1:75:A:SER:HB2	9	0.11
(1,655)	1:75:A:SER:H	1:75:A:SER:HB3	9	0.11
(1,634)	1:69:A:THR:HA	1:72:A:ARG:H	7	0.11
(1,633)	1:72:A:ARG:H	1:73:A:GLU:HA	13	0.11
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	7	0.11
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	8	0.11
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	13	0.11
(1,626)	1:71:A:ALA:H	1:72:A:ARG:H	17	0.11
(1,598)	1:62:A:PHE:HA	1:66:A:GLY:H	8	0.11
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	4	0.11
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	15	0.11
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:62:A:PHE:HD1	1:64:A:ASP:H	8	0.11
(1,580)	1:62:A:PHE:HD2	1:64:A:ASP:H	8	0.11
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	16	0.11
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	17	0.11
(1,575)	1:64:A:ASP:H	1:65:A:VAL:HA	19	0.11
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	4	0.11
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	4	0.11
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD1	12	0.11
(1,569)	1:62:A:PHE:H	1:62:A:PHE:HD2	12	0.11
(1,557)	1:29:A:LEU:HA	1:61:A:ASN:H	3	0.11
(1,551)	1:59:A:THR:HG1	1:61:A:ASN:H	16	0.11
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	17	0.11
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	17	0.11
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	17	0.11
(1,542)	1:58:A:ALA:HB1	1:59:A:THR:H	9	0.11
(1,542)	1:58:A:ALA:HB2	1:59:A:THR:H	9	0.11
(1,542)	1:58:A:ALA:HB3	1:59:A:THR:H	9	0.11
(1,520)	1:56:A:GLY:HA3	1:57:A:ASP:H	18	0.11
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	5	0.11
(1,495)	1:51:A:ARG:HE	1:52:A:GLU:H	20	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	1	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	1	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	1	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	3	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	3	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	3	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	7	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	7	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	7	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	8	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	8	0.11
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	8	0.11
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	3	0.11
(1,456)	1:46:A:GLY:HA3	1:49:A:VAL:H	17	0.11
(1,455)	1:46:A:GLY:H	1:48:A:GLU:HG2	3	0.11
(1,447)	1:40:A:LEU:HD11	1:46:A:GLY:H	16	0.11
(1,447)	1:40:A:LEU:HD12	1:46:A:GLY:H	16	0.11
(1,447)	1:40:A:LEU:HD13	1:46:A:GLY:H	16	0.11
(1,447)	1:40:A:LEU:HD21	1:46:A:GLY:H	16	0.11
(1,447)	1:40:A:LEU:HD22	1:46:A:GLY:H	16	0.11
(1,447)	1:40:A:LEU:HD23	1:46:A:GLY:H	16	0.11
(1,410)	1:22:A:SER:HB3	1:41:A:GLU:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	9	0.11
(1,405)	1:38:A:LYS:H	1:41:A:GLU:H	15	0.11
(1,402)	1:25:A:THR:HB	1:40:A:LEU:H	2	0.11
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD1	18	0.11
(1,382)	1:39:A:PHE:H	1:39:A:PHE:HD2	18	0.11
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD11	20	0.11
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD12	20	0.11
(1,372)	1:37:A:THR:H	1:40:A:LEU:HD13	20	0.11
(1,371)	1:37:A:THR:H	1:38:A:LYS:H	5	0.11
(1,366)	1:26:A:TRP:HD1	1:37:A:THR:H	5	0.11
(1,364)	1:25:A:THR:HB	1:37:A:THR:H	13	0.11
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	13	0.11
(1,362)	1:25:A:THR:HA	1:37:A:THR:H	14	0.11
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	12	0.11
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	3	0.11
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	7	0.11
(1,352)	1:36:A:LEU:H	1:37:A:THR:HB	19	0.11
(1,347)	1:34:A:TYR:HB3	1:36:A:LEU:H	7	0.11
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG21	19	0.11
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG22	19	0.11
(1,339)	1:35:A:ASP:H	1:79:A:ILE:HG23	19	0.11
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG21	12	0.11
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG22	12	0.11
(1,334)	1:35:A:ASP:H	1:80:A:ILE:HG23	12	0.11
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	8	0.11
(1,305)	1:26:A:TRP:HB2	1:34:A:TYR:H	19	0.11
(1,297)	1:33:A:VAL:H	1:82:A:GLU:HA	8	0.11
(1,280)	1:31:A:HIS:HB2	1:32:A:LYS:H	13	0.11
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	11	0.11
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	4	0.11
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	7	0.11
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	14	0.11
(1,256)	1:30:A:HIS:H	1:30:A:HIS:HB3	20	0.11
(1,252)	1:30:A:HIS:H	1:30:A:HIS:HD1	8	0.11
(1,248)	1:29:A:LEU:H	1:30:A:HIS:HB3	6	0.11
(1,233)	1:13:A:LEU:HD11	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD12	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD13	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD21	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD22	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD23	1:28:A:ILE:H	11	0.11
(1,233)	1:13:A:LEU:HD11	1:28:A:ILE:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:13:A:LEU:HD12	1:28:A:ILE:H	15	0.11
(1,233)	1:13:A:LEU:HD13	1:28:A:ILE:H	15	0.11
(1,233)	1:13:A:LEU:HD21	1:28:A:ILE:H	15	0.11
(1,233)	1:13:A:LEU:HD22	1:28:A:ILE:H	15	0.11
(1,233)	1:13:A:LEU:HD23	1:28:A:ILE:H	15	0.11
(1,226)	1:28:A:ILE:H	1:28:A:ILE:HB	19	0.11
(1,217)	1:16:A:ILE:HD11	1:27:A:VAL:H	6	0.11
(1,217)	1:16:A:ILE:HD12	1:27:A:VAL:H	6	0.11
(1,217)	1:16:A:ILE:HD13	1:27:A:VAL:H	6	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD21	3	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD22	3	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD23	3	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD11	3	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD12	3	0.11
(1,216)	1:27:A:VAL:H	1:36:A:LEU:HD13	3	0.11
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG21	19	0.11
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG22	19	0.11
(1,211)	1:27:A:VAL:H	1:27:A:VAL:HG23	19	0.11
(1,204)	1:26:A:TRP:H	1:36:A:LEU:HG	14	0.11
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	3	0.11
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	4	0.11
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	11	0.11
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	18	0.11
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	8	0.11
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	16	0.11
(1,191)	1:25:A:THR:H	1:37:A:THR:H	13	0.11
(1,181)	1:23:A:LYS:HD3	1:24:A:SER:H	1	0.11
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG2	17	0.11
(1,165)	1:23:A:LYS:H	1:23:A:LYS:HG3	17	0.11
(1,161)	1:22:A:SER:HG	1:23:A:LYS:H	5	0.11
(1,158)	1:22:A:SER:H	1:24:A:SER:H	17	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	10	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	10	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	10	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD21	14	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD22	14	0.11
(1,154)	1:22:A:SER:H	1:40:A:LEU:HD23	14	0.11
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD2	1	0.11
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD3	1	0.11
(1,139)	1:21:A:ASP:H	1:23:A:LYS:HD3	4	0.11
(1,120)	1:16:A:ILE:H	1:16:A:ILE:HD11	11	0.11
(1,120)	1:16:A:ILE:H	1:16:A:ILE:HD12	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:16:A:ILE:H	1:16:A:ILE:HD13	11	0.11
(1,119)	1:16:A:ILE:H	1:19:A:HIS:HD1	17	0.11
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	12	0.11
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	14	0.11
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	1	0.11
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	8	0.11
(1,112)	1:13:A:LEU:HA	1:15:A:GLU:H	9	0.11
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	1	0.11
(1,85)	1:12:A:THR:HG1	1:14:A:GLU:H	18	0.11
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	9	0.11
(1,76)	1:13:A:LEU:H	1:13:A:LEU:HG	11	0.11
(1,71)	1:12:A:THR:H	1:87:A:ASP:HB2	8	0.11
(1,68)	1:12:A:THR:H	1:16:A:ILE:H	18	0.11
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	5	0.11
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	16	0.11
(1,62)	1:11:A:TYR:HB2	1:12:A:THR:H	4	0.11
(1,62)	1:11:A:TYR:HB3	1:12:A:THR:H	4	0.11
(1,62)	1:11:A:TYR:HB2	1:12:A:THR:H	8	0.11
(1,62)	1:11:A:TYR:HB3	1:12:A:THR:H	8	0.11
(1,62)	1:11:A:TYR:HB2	1:12:A:THR:H	15	0.11
(1,62)	1:11:A:TYR:HB3	1:12:A:THR:H	15	0.11
(1,62)	1:11:A:TYR:HB2	1:12:A:THR:H	19	0.11
(1,62)	1:11:A:TYR:HB3	1:12:A:THR:H	19	0.11
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD1	14	0.11
(1,43)	1:10:A:TYR:H	1:10:A:TYR:HD2	14	0.11
(1,39)	1:9:A:LYS:HD2	1:10:A:TYR:H	3	0.11
(1,39)	1:9:A:LYS:HD3	1:10:A:TYR:H	3	0.11
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	10	0.11
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	15	0.11
(1,24)	1:6:A:LYS:HB3	1:8:A:VAL:H	14	0.11
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	2	0.11
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	2	0.11
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	2	0.11
(1,12)	1:4:A:SER:H	1:6:A:LYS:H	18	0.11
(3,18)	1:28:A:ILE:O	1:58:A:ALA:H	10	0.1
(3,1)	1:25:A:THR:O	1:36:A:LEU:H	18	0.1
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	11	0.1
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	11	0.1
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	11	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	11	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	11	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB1	13	0.1
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB2	13	0.1
(2,86)	1:39:A:PHE:HE1	1:58:A:ALA:HB3	13	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB1	13	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB2	13	0.1
(2,86)	1:39:A:PHE:HE2	1:58:A:ALA:HB3	13	0.1
(2,58)	1:81:A:GLY:H	1:83:A:LEU:H	12	0.1
(2,37)	1:43:A:TRP:HE3	1:67:A:PHE:H	1	0.1
(1,1087)	1:50:A:LEU:HA	1:61:A:ASN:HD21	8	0.1
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD1	11	0.1
(1,1048)	1:32:A:LYS:HA	1:34:A:TYR:HD2	11	0.1
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	17	0.1
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	17	0.1
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG21	1:34:A:TYR:HD2	20	0.1
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG22	1:34:A:TYR:HD2	20	0.1
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG23	1:34:A:TYR:HD2	20	0.1
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG11	1:34:A:TYR:HD2	20	0.1
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG12	1:34:A:TYR:HD2	20	0.1
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD1	20	0.1
(1,1044)	1:33:A:VAL:HG13	1:34:A:TYR:HD2	20	0.1
(1,1018)	1:16:A:ILE:HD11	1:26:A:TRP:HE3	16	0.1
(1,1018)	1:16:A:ILE:HD12	1:26:A:TRP:HE3	16	0.1
(1,1018)	1:16:A:ILE:HD13	1:26:A:TRP:HE3	16	0.1
(1,1016)	1:16:A:ILE:HA	1:26:A:TRP:HE3	11	0.1
(1,1008)	1:26:A:TRP:HA	1:26:A:TRP:HD1	4	0.1
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	5	0.1
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	5	0.1
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	5	0.1
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA3	9	0.1
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA3	9	0.1
(1,985)	1:11:A:TYR:HE1	1:81:A:GLY:HA2	9	0.1
(1,985)	1:11:A:TYR:HE2	1:81:A:GLY:HA2	9	0.1
(1,971)	1:83:A:LEU:HD11	1:86:A:ASP:HA	8	0.1
(1,971)	1:83:A:LEU:HD12	1:86:A:ASP:HA	8	0.1
(1,971)	1:83:A:LEU:HD13	1:86:A:ASP:HA	8	0.1
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	3	0.1
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	3	0.1
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA2	14	0.1
(1,956)	1:80:A:ILE:HB	1:81:A:GLY:HA3	14	0.1
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	8	0.1
(1,946)	1:97:A:THR:HA	1:98:A:LEU:H	13	0.1
(1,908)	1:93:A:LYS:H	1:94:A:PRO:HA	10	0.1
(1,896)	1:91:A:ILE:HG13	1:92:A:ALA:H	7	0.1
(1,892)	1:91:A:ILE:HB	1:92:A:ALA:H	15	0.1
(1,855)	1:88:A:ARG:H	1:90:A:LYS:H	14	0.1
(1,841)	1:86:A:ASP:HA	1:89:A:SER:H	13	0.1
(1,829)	1:31:A:HIS:HA	1:88:A:ARG:H	1	0.1
(1,825)	1:86:A:ASP:HA	1:88:A:ARG:H	10	0.1
(1,816)	1:87:A:ASP:H	1:87:A:ASP:HB3	14	0.1
(1,812)	1:86:A:ASP:HA	1:87:A:ASP:H	13	0.1
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	1	0.1
(1,800)	1:86:A:ASP:H	1:87:A:ASP:HA	20	0.1
(1,795)	1:85:A:PRO:HG2	1:86:A:ASP:H	6	0.1
(1,795)	1:85:A:PRO:HG3	1:86:A:ASP:H	6	0.1
(1,784)	1:13:A:LEU:H	1:84:A:HIS:H	3	0.1
(1,781)	1:11:A:TYR:HA	1:84:A:HIS:H	8	0.1
(1,780)	1:11:A:TYR:H	1:84:A:HIS:H	17	0.1
(1,765)	1:10:A:TYR:HA	1:83:A:LEU:H	1	0.1
(1,757)	1:11:A:TYR:HE1	1:82:A:GLU:H	18	0.1
(1,757)	1:11:A:TYR:HE2	1:82:A:GLU:H	18	0.1
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG21	19	0.1
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG22	19	0.1
(1,725)	1:80:A:ILE:H	1:80:A:ILE:HG23	19	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	9	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	9	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	9	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	14	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	14	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD11	16	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD12	16	0.1
(1,714)	1:79:A:ILE:H	1:79:A:ILE:HD13	16	0.1
(1,691)	1:76:A:LYS:HA	1:78:A:TYR:H	2	0.1
(1,687)	1:35:A:ASP:HB3	1:78:A:TYR:H	4	0.1
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD2	19	0.1
(1,670)	1:76:A:LYS:H	1:77:A:LYS:HD3	19	0.1
(1,651)	1:74:A:LEU:H	1:75:A:SER:H	19	0.1
(1,613)	1:67:A:PHE:H	1:71:A:ALA:H	16	0.1
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	8	0.1
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	16	0.1
(1,596)	1:65:A:VAL:H	1:66:A:GLY:H	20	0.1
(1,587)	1:62:A:PHE:HA	1:65:A:VAL:H	14	0.1
(1,584)	1:62:A:PHE:H	1:65:A:VAL:H	8	0.1
(1,583)	1:64:A:ASP:H	1:65:A:VAL:H	16	0.1
(1,566)	1:59:A:THR:HA	1:62:A:PHE:H	14	0.1
(1,561)	1:61:A:ASN:H	1:64:A:ASP:H	5	0.1
(1,553)	1:60:A:GLU:HA	1:61:A:ASN:H	12	0.1
(1,545)	1:59:A:THR:H	1:59:A:THR:HG21	20	0.1
(1,545)	1:59:A:THR:H	1:59:A:THR:HG22	20	0.1
(1,545)	1:59:A:THR:H	1:59:A:THR:HG23	20	0.1
(1,542)	1:58:A:ALA:HB1	1:59:A:THR:H	18	0.1
(1,542)	1:58:A:ALA:HB2	1:59:A:THR:H	18	0.1
(1,542)	1:58:A:ALA:HB3	1:59:A:THR:H	18	0.1
(1,537)	1:28:A:ILE:H	1:59:A:THR:H	17	0.1
(1,504)	1:51:A:ARG:HA	1:53:A:GLN:H	18	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	2	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	2	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	2	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG21	11	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG22	11	0.1
(1,466)	1:49:A:VAL:H	1:49:A:VAL:HG23	11	0.1
(1,434)	1:40:A:LEU:HB2	1:43:A:TRP:H	16	0.1
(1,434)	1:40:A:LEU:HB3	1:43:A:TRP:H	16	0.1
(1,424)	1:38:A:LYS:HA	1:42:A:GLU:H	18	0.1
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD11	8	0.1
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD12	8	0.1
(1,392)	1:40:A:LEU:H	1:40:A:LEU:HD13	8	0.1
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE1	19	0.1
(1,383)	1:39:A:PHE:H	1:78:A:TYR:HE2	19	0.1
(1,379)	1:38:A:LYS:HE3	1:39:A:PHE:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:36:A:LEU:HB2	1:38:A:LYS:H	20	0.1
(1,377)	1:36:A:LEU:HB3	1:38:A:LYS:H	20	0.1
(1,359)	1:25:A:THR:HG1	1:37:A:THR:H	20	0.1
(1,335)	1:27:A:VAL:HG21	1:35:A:ASP:H	5	0.1
(1,335)	1:27:A:VAL:HG22	1:35:A:ASP:H	5	0.1
(1,335)	1:27:A:VAL:HG23	1:35:A:ASP:H	5	0.1
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD1	7	0.1
(1,304)	1:34:A:TYR:H	1:34:A:TYR:HD2	7	0.1
(1,294)	1:11:A:TYR:HD1	1:33:A:VAL:H	13	0.1
(1,294)	1:11:A:TYR:HD2	1:33:A:VAL:H	13	0.1
(1,287)	1:29:A:LEU:HD21	1:33:A:VAL:H	10	0.1
(1,287)	1:29:A:LEU:HD22	1:33:A:VAL:H	10	0.1
(1,287)	1:29:A:LEU:HD23	1:33:A:VAL:H	10	0.1
(1,279)	1:31:A:HIS:H	1:32:A:LYS:H	11	0.1
(1,274)	1:28:A:ILE:HB	1:32:A:LYS:H	7	0.1
(1,240)	1:28:A:ILE:HB	1:29:A:LEU:H	17	0.1
(1,226)	1:28:A:ILE:H	1:28:A:ILE:HB	2	0.1
(1,223)	1:27:A:VAL:HB	1:28:A:ILE:H	8	0.1
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	6	0.1
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	7	0.1
(1,206)	1:26:A:TRP:HD1	1:27:A:VAL:H	20	0.1
(1,199)	1:26:A:TRP:H	1:26:A:TRP:HD1	13	0.1
(1,192)	1:16:A:ILE:HB	1:26:A:TRP:H	1	0.1
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD2	19	0.1
(1,148)	1:21:A:ASP:H	1:23:A:LYS:HD3	19	0.1
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	5	0.1
(1,114)	1:15:A:GLU:H	1:16:A:ILE:H	13	0.1
(1,103)	1:12:A:THR:HG1	1:15:A:GLU:H	18	0.1
(1,82)	1:13:A:LEU:H	1:83:A:LEU:HA	5	0.1
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	6	0.1
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	11	0.1
(1,66)	1:12:A:THR:H	1:13:A:LEU:H	14	0.1
(1,40)	1:9:A:LYS:HB2	1:10:A:TYR:H	14	0.1
(1,40)	1:9:A:LYS:HB3	1:10:A:TYR:H	14	0.1
(1,28)	1:9:A:LYS:H	1:81:A:GLY:HA2	6	0.1
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD2	3	0.1
(1,22)	1:6:A:LYS:H	1:6:A:LYS:HD3	3	0.1
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ1	6	0.1
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ2	6	0.1
(1,19)	1:6:A:LYS:H	1:6:A:LYS:HZ3	6	0.1
(1,16)	1:4:A:SER:HB3	1:6:A:LYS:H	16	0.1

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

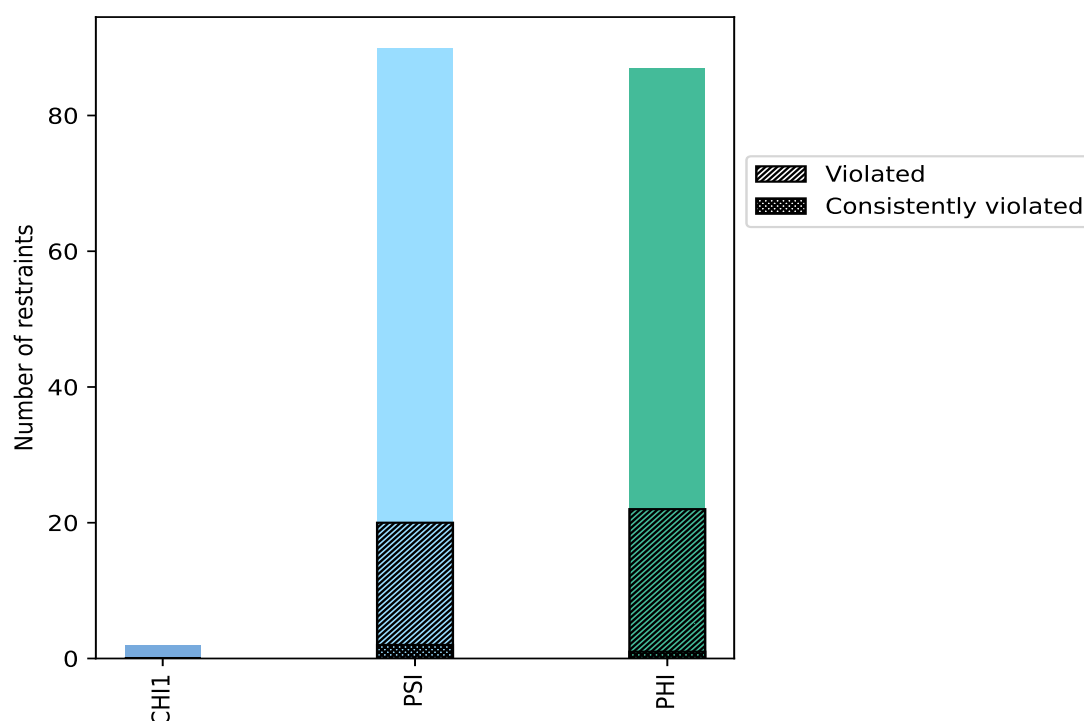
10.1 Summary of dihedral-angle violations [i](#)

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
CHI1	2	1.1	0	0.0	0.0	0	0.0	0.0
PSI	90	50.3	20	22.2	11.2	2	2.2	1.1
PHI	87	48.6	22	25.3	12.3	1	1.1	0.6
Total	179	100.0	42	23.5	23.5	3	1.7	1.7

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](#)



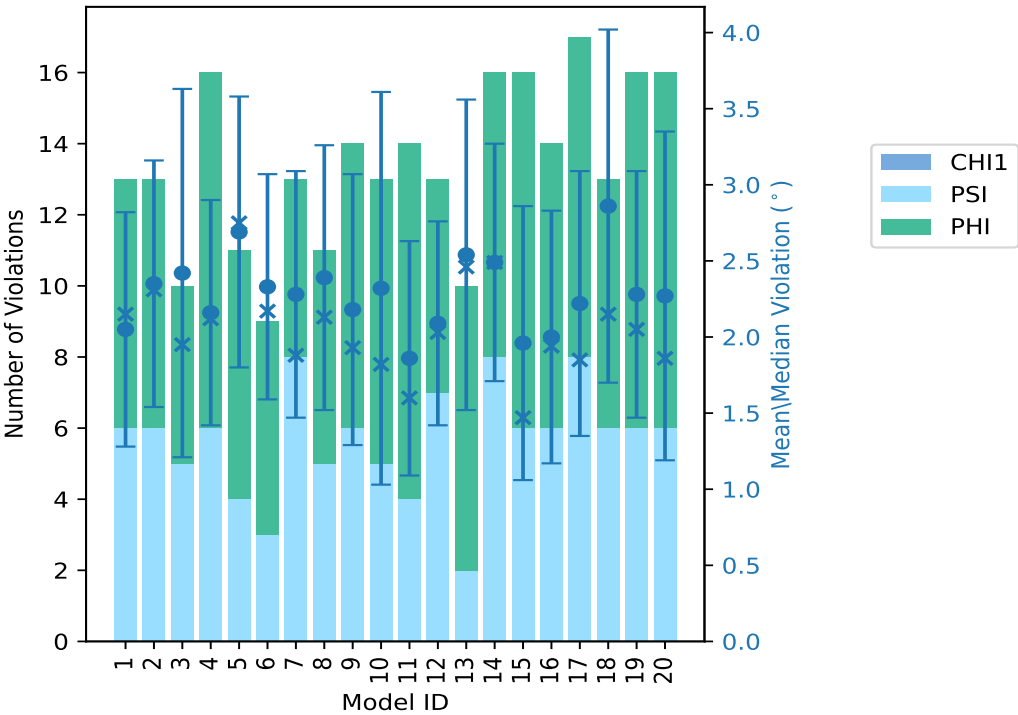
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 (°)
	CHI1	PSI	PHI	Total				
1	0	6	7	13	2.05	3.32	0.77	2.15
2	0	6	7	13	2.35	3.57	0.81	2.31
3	0	5	5	10	2.42	4.22	1.21	1.95
4	0	6	10	16	2.16	4.19	0.74	2.12
5	0	4	7	11	2.69	4.26	0.89	2.75
6	0	3	6	9	2.33	3.77	0.74	2.17
7	0	8	5	13	2.28	3.79	0.81	1.88
8	0	5	6	11	2.39	3.61	0.87	2.13
9	0	6	8	14	2.18	3.81	0.89	1.93
10	0	5	8	13	2.32	4.88	1.29	1.82
11	0	4	10	14	1.86	3.96	0.77	1.6
12	0	7	6	13	2.09	3.38	0.67	2.03
13	0	2	8	10	2.54	4.28	1.02	2.46
14	0	8	8	16	2.49	4.34	0.78	2.49
15	0	6	10	16	1.96	3.62	0.9	1.47
16	0	6	8	14	2.0	4.0	0.83	1.94
17	0	8	9	17	2.22	4.34	0.87	1.85
18	0	6	7	13	2.86	4.95	1.16	2.15
19	0	6	10	16	2.28	3.86	0.81	2.05
20	0	6	10	16	2.27	4.92	1.08	1.86

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints				Fraction of the ensemble	
CHI1	PSI	PHI	Total	Count ¹	%
0	5	9	14	1	5.0
0	3	1	4	2	10.0
0	1	1	2	3	15.0
0	2	0	2	4	20.0
0	3	1	4	5	25.0
0	1	1	2	6	30.0
0	0	0	0	7	35.0
0	0	0	0	8	40.0
0	0	0	0	9	45.0
0	3	2	5	10	50.0
0	0	0	0	11	55.0

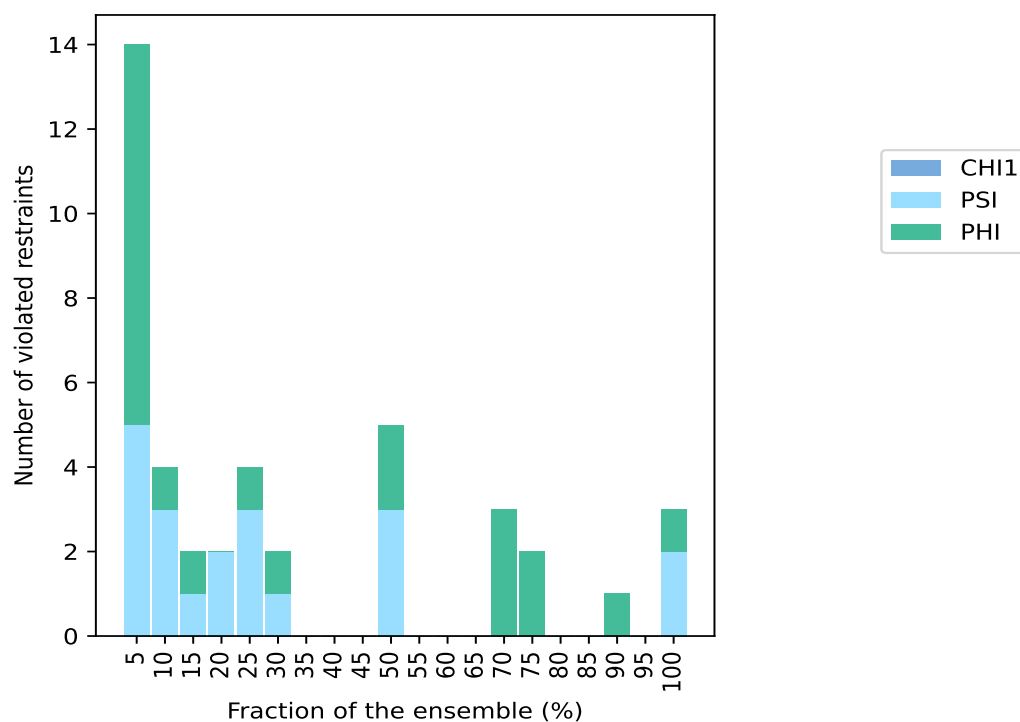
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Number of violated restraints				Fraction of the ensemble	
CHI1	PSI	PHI	Total	Count ¹	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	3	3	14	70.0
0	0	2	2	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	1	1	18	90.0
0	0	0	0	19	95.0
0	2	1	3	20	100.0

¹ Number of models with violations

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

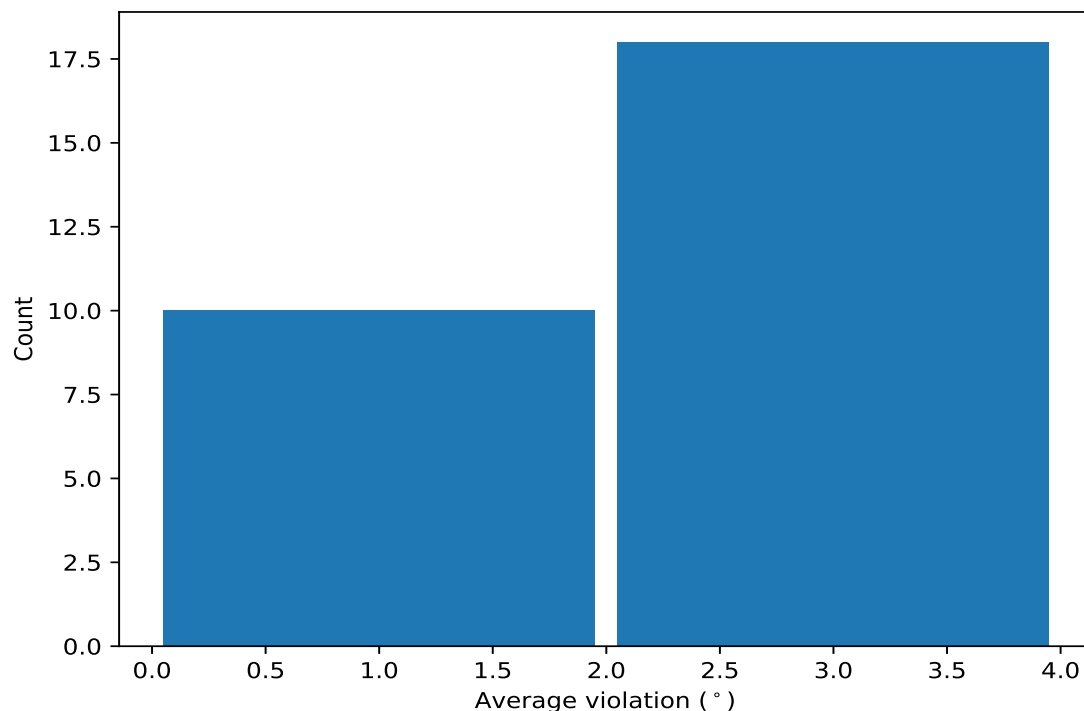


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	20	3.31	0.96	3.38
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	20	3.15	0.78	3.1
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	20	2.46	0.59	2.39
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	18	2.61	0.93	2.25
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	15	2.08	0.82	1.76
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	15	2.07	0.89	1.86
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	14	2.31	1.05	1.9
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	14	2.14	0.88	2.16
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	14	2.03	0.64	1.91
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	10	2.09	1.2	1.54
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	10	2.06	0.75	1.92
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	10	2.0	0.76	1.92
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	10	1.98	0.63	1.81
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	10	1.78	0.39	1.83
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	6	1.9	0.7	1.88
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	6	1.68	0.52	1.5
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	5	2.52	1.36	1.63
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	5	1.78	0.34	1.7
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	5	1.7	0.45	1.52
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	5	1.42	0.32	1.24

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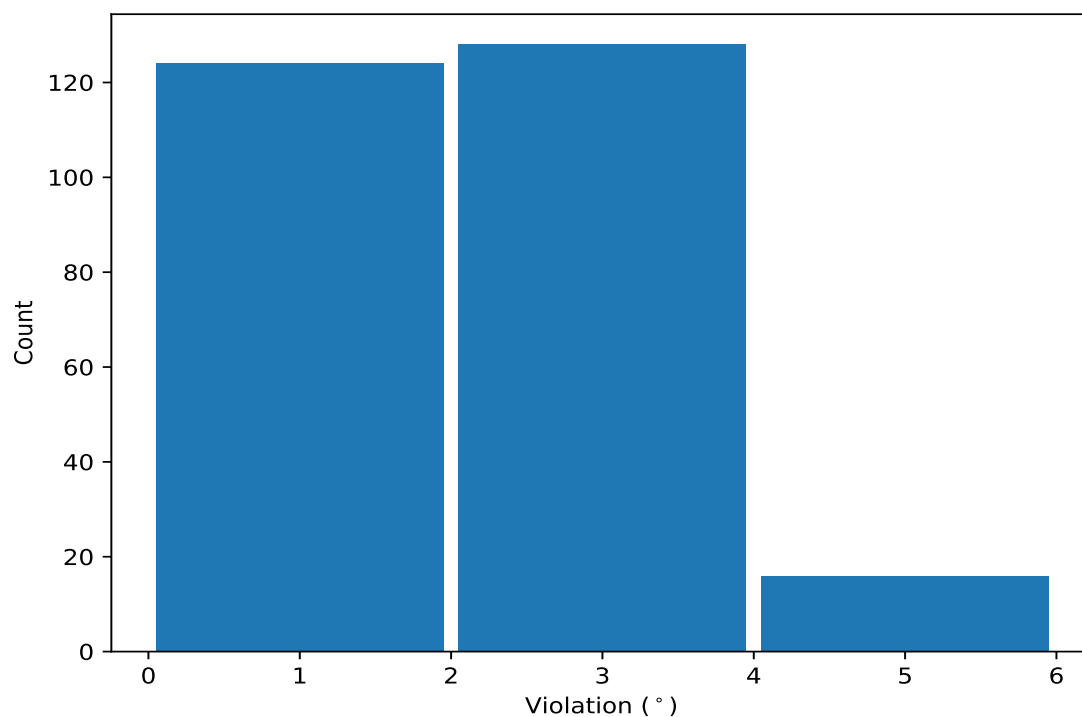
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,34)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:LYS:N	4	2.19	0.65	2.08
(1,127)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:THR:N	4	2.01	0.51	1.94
(1,177)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:THR:N	3	2.47	0.88	2.31
(1,146)	1:77:A:LYS:C	1:78:A:TYR:N	1:78:A:TYR:CA	1:78:A:TYR:C	3	1.91	0.89	1.29
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:LYS:N	2	2.93	1.29	2.93
(1,176)	1:95:A:SER:C	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	2	2.44	0.56	2.44
(1,174)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:PRO:N	2	1.96	0.21	1.96
(1,175)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:SER:N	2	1.52	0.12	1.52

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 (°)
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	18	4.95
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	20	4.92
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	10	4.88
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	10	4.7
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	20	4.61
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	18	4.58
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	17	4.34
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	14	4.34
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	13	4.28
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	5	4.26
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:LYS:N	3	4.22
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	3	4.21
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	4	4.19
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	18	4.16
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	13	4.1
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	16	4.0
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	11	3.96
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	18	3.93
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	5	3.9
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	19	3.86
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	9	3.81
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	7	3.79
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	6	3.77
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	3	3.67
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	14	3.66
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	18	3.63
(1,177)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:THR:N	7	3.62
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	9	3.62
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	15	3.62
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	8	3.61
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	15	3.6
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	19	3.58
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	2	3.57
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	8	3.55
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	2	3.52
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	7	3.49
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	8	3.43
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	14	3.4
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	12	3.38
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	12	3.37
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	17	3.35
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	1	3.32
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	9	3.28
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	4	3.26
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	19	3.26
(1,173)	1:92:A:ALA:C	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	16	3.25
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	17	3.23
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	19	3.21
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	3	3.18
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	2	3.18
(1,146)	1:77:A:LYS:C	1:78:A:TYR:N	1:78:A:TYR:CA	1:78:A:TYR:C	5	3.17
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	5	3.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	9	3.14
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	2	3.14
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	20	3.12
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	13	3.12
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	5	3.07
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	17	3.07
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	10	3.06
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1	3.04
(1,34)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:LYS:N	15	3.04
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	8	3.03
(1,176)	1:95:A:SER:C	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	15	2.99
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	15	2.97
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	10	2.96
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	1	2.96
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	10	2.93
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	14	2.91
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	6	2.91
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	14	2.88
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	11	2.87
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	6	2.87
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	13	2.81
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	17	2.8
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	19	2.76
(1,127)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:THR:N	8	2.76
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	13	2.76
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	5	2.75
(1,71)	1:37:A:THR:C	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	17	2.69
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	16	2.66
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	7	2.66
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	14	2.66
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	1	2.66
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	2	2.65
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	20	2.65
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	6	2.64
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	18	2.63
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	2	2.61
(1,34)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:LYS:N	10	2.6
(1,136)	1:72:A:ARG:C	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	12	2.58
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	14	2.54
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	19	2.51
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	14	2.49
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	11	2.49
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	14	2.48
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1	2.46
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	20	2.45
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	4	2.4
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	4	2.4
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	4	2.37
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	4	2.37
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	9	2.36
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	12	2.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	16	2.34
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	4	2.33
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	5	2.32
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	5	2.32
(1,177)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:THR:N	17	2.31
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	2	2.31
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	7	2.27
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	1	2.26
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	20	2.24
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	11	2.23
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	16	2.21
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	17	2.21
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	14	2.21
(1,127)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:THR:N	9	2.19
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	20	2.17
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	6	2.17
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	13	2.17
(1,174)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:PRO:N	2	2.16
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	1	2.15
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	12	2.15
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	18	2.15
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	3	2.14
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	16	2.14
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	19	2.13
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	8	2.13
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	4	2.13
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	4	2.1
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	18	2.1
(1,1)	1:2:A:GLU:C	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	19	2.08
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	18	2.07
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	18	2.06
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	13	2.06
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	14	2.05
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	4	2.04
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	7	2.04
(1,145)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:TYR:N	12	2.03
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	9	2.03
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	12	2.03
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	16	2.02
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	19	2.02
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	6	2.0
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	11	1.97
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	19	1.92
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	18	1.91
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	8	1.91
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	2	1.89
(1,176)	1:95:A:SER:C	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	4	1.88
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	7	1.88
(1,117)	1:62:A:PHE:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	20	1.87
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	12	1.87
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	19	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	7	1.86
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	7	1.86
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	19	1.86
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	16	1.86
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	17	1.85
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	20	1.84
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	9	1.83
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	20	1.83
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	10	1.82
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	15	1.78
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	14	1.78
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	3	1.76
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	8	1.76
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	17	1.76
(1,174)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:PRO:N	9	1.75
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	4	1.75
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	5	1.74
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	20	1.73
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	12	1.73
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	11	1.73
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	19	1.71
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1	1.71
(1,127)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:THR:N	12	1.7
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	14	1.7
(1,97)	1:52:A:GLU:C	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	14	1.69
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	17	1.67
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	20	1.66
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	15	1.65
(1,175)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:SER:N	17	1.64
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	12	1.64
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:LYS:N	14	1.64
(1,86)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:GLY:N	6	1.63
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	18	1.63
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	11	1.63
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	5	1.61
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	10	1.59
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	4	1.59
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	7	1.59
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	11	1.58
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	11	1.58
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	6	1.57
(1,34)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:LYS:N	7	1.57
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	2	1.57
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	20	1.57
(1,34)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:LYS:N	17	1.55
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	9	1.53
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	17	1.52
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	15	1.52
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	8	1.5
(1,177)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:THR:N	20	1.49
(1,129)	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	1:70:A:ASP:N	7	1.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	3	1.47
(1,54)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:HIS:N	7	1.47
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	16	1.46
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	14	1.46
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	13	1.44
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	17	1.44
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	18	1.43
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	13	1.42
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	15	1.42
(1,148)	1:78:A:TYR:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	15	1.41
(1,127)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:THR:N	19	1.41
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	15	1.41
(1,17)	1:10:A:TYR:C	1:11:A:TYR:N	1:11:A:TYR:CA	1:11:A:TYR:C	2	1.41
(1,175)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:SER:N	11	1.39
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	6	1.38
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	5	1.36
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	15	1.36
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	9	1.36
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	4	1.35
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	1	1.34
(1,13)	1:8:A:VAL:C	1:9:A:LYS:N	1:9:A:LYS:CA	1:9:A:LYS:C	19	1.34
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	8	1.33
(1,53)	1:28:A:ILE:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	9	1.33
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	3	1.3
(1,170)	1:91:A:ILE:N	1:91:A:ILE:CA	1:91:A:ILE:C	1:92:A:ALA:N	1	1.29
(1,146)	1:77:A:LYS:C	1:78:A:TYR:N	1:78:A:TYR:CA	1:78:A:TYR:C	1	1.29
(1,98)	1:53:A:GLN:N	1:53:A:GLN:CA	1:53:A:GLN:C	1:54:A:ALA:N	2	1.29
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	8	1.28
(1,67)	1:35:A:ASP:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	17	1.27
(1,146)	1:77:A:LYS:C	1:78:A:TYR:N	1:78:A:TYR:CA	1:78:A:TYR:C	15	1.26
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	13	1.25
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	9	1.25
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	16	1.24
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	10	1.24
(1,16)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:TYR:N	16	1.24
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	11	1.24
(1,36)	1:20:A:LYS:N	1:20:A:LYS:CA	1:20:A:LYS:C	1:21:A:ASP:N	4	1.23
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	16	1.23
(1,65)	1:34:A:TYR:C	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	2	1.22
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	11	1.21
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	16	1.2
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	12	1.19
(1,44)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:THR:N	16	1.18
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	11	1.17
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	4	1.16
(1,165)	1:88:A:ARG:C	1:89:A:SER:N	1:89:A:SER:CA	1:89:A:SER:C	12	1.16
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	10	1.16
(1,151)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLU:N	10	1.13
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	15	1.13
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	1	1.13
(1,66)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:LEU:N	3	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:18:A:LYS:N	1:18:A:LYS:CA	1:18:A:LYS:C	1:19:A:HIS:N	17	1.12
(1,84)	1:44:A:PRO:N	1:44:A:PRO:CA	1:44:A:PRO:C	1:45:A:GLY:N	15	1.11
(1,61)	1:32:A:LYS:C	1:33:A:VAL:N	1:33:A:VAL:CA	1:33:A:VAL:C	20	1.1
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	9	1.1
(1,150)	1:80:A:ILE:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	10	1.08
(1,124)	1:67:A:PHE:N	1:67:A:PHE:CA	1:67:A:PHE:C	1:68:A:SER:N	3	1.08
(1,15)	1:9:A:LYS:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	15	1.08
(1,111)	1:59:A:THR:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	10	1.05
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	20	1.04
(1,121)	1:64:A:ASP:C	1:65:A:VAL:N	1:65:A:VAL:CA	1:65:A:VAL:C	11	1.03
(1,9)	1:6:A:LYS:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	19	1.02
(1,91)	1:49:A:VAL:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1	1.01