



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:14 AM UTC

PDB ID : 9GE9 / pdb_00009ge9
BMRB ID : 34950
Title : Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR) at 277K
Authors : Horvath, D.
Deposited on : 2024-08-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

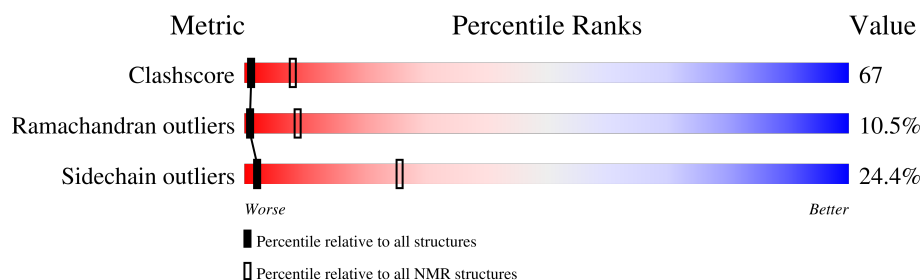
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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	25	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:24 (19)	0.42	5

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4, 5, 6, 7, 8, 9
2	3, 10
Single-model clusters	1

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 390 atoms, of which 193 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR).

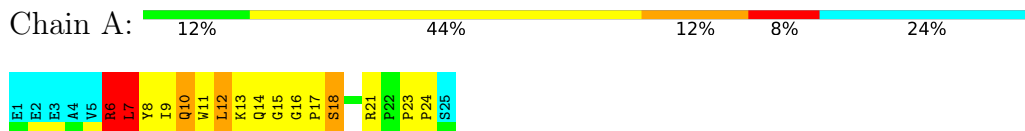
Mol	Chain	Residues	Atoms					Trace
1	A	25	Total	C	H	N	O	0
			390	124	193	35	38	

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: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)

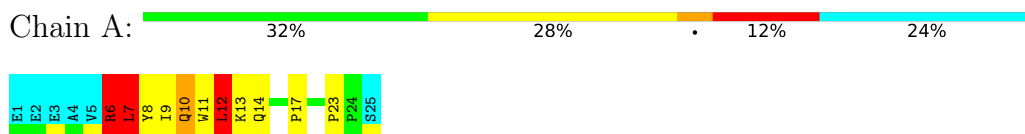


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

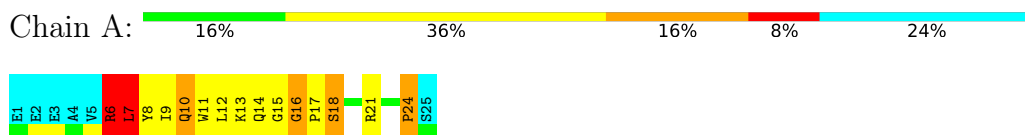
4.2.1 Score per residue for model 1

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



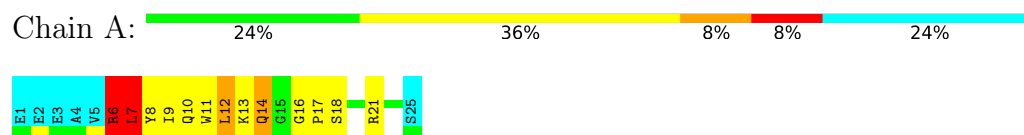
4.2.2 Score per residue for model 2

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



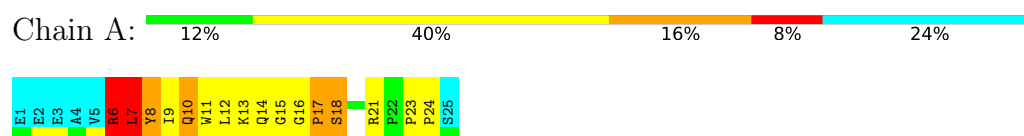
4.2.3 Score per residue for model 3

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



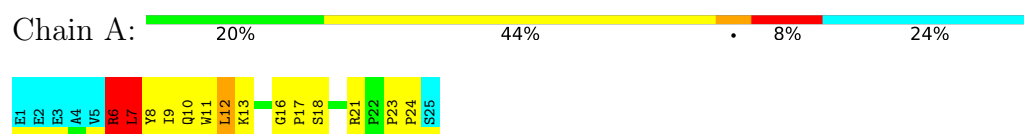
4.2.4 Score per residue for model 4

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



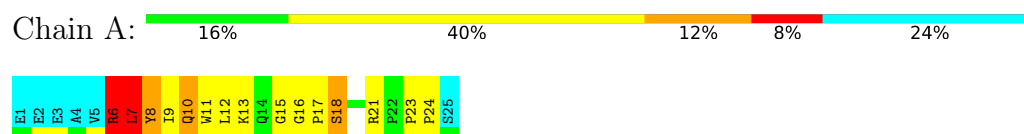
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



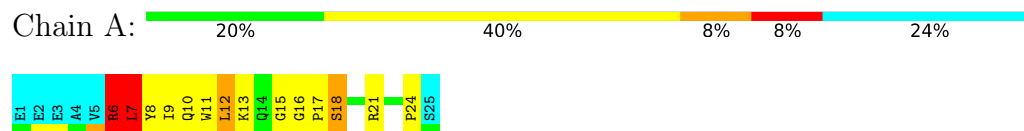
4.2.6 Score per residue for model 6

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



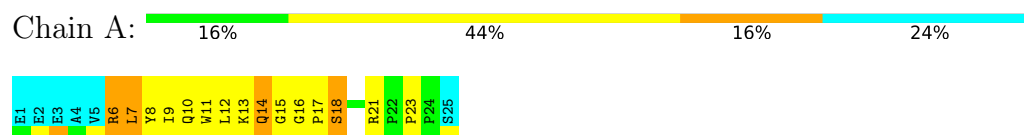
4.2.7 Score per residue for model 7

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



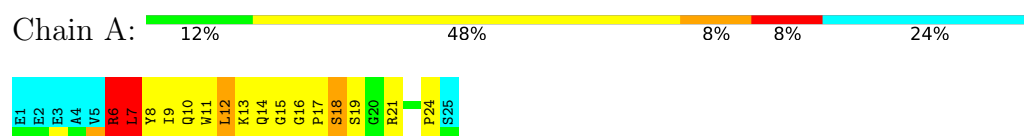
4.2.8 Score per residue for model 8

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



4.2.9 Score per residue for model 9

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



4.2.10 Score per residue for model 10

- Molecule 1: Trp-cage fortified Tc5b-Exenatide chimera (Ex-4-Tc5bQR)



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CcpNmr Analysis Assign	refinement	2.4.1.
ARIA2alpha	structure calculation	2.3.1.

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	168
Number of shifts mapped to atoms	168
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%

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	1.18±0.07	0±0/158 (0.0± 0.0%)	1.53±0.09	3±1/216 (1.2± 0.4%)
All	All	1.18	0/1580 (0.0%)	1.54	27/2160 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.6±0.5
All	All	0	6

There are no bond-length outliers.

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	7	LEU	N-CA-CB	-7.24	101.27	110.90	10	10
1	A	6	ARG	CA-C-N	7.04	129.59	120.44	8	1
1	A	6	ARG	C-N-CA	7.04	129.59	120.44	8	1
1	A	12	LEU	N-CA-CB	-6.26	100.20	110.40	1	1
1	A	6	ARG	N-CA-C	-5.99	105.63	113.12	9	9
1	A	6	ARG	CA-C-O	5.22	125.46	119.35	7	5

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	ARG	Sidechain	6

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	151	154	154	20±3
All	All	1510	1540	1540	204

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 67.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:CZ2	1:A:17:PRO:HD3	1.08	1.83	4	1
1:A:11:TRP:CH2	1:A:17:PRO:HD3	0.85	2.06	4	2
1:A:7:LEU:HD13	1:A:8:TYR:N	0.84	1.88	9	9
1:A:9:ILE:O	1:A:13:LYS:HG2	0.73	1.83	8	7
1:A:12:LEU:HD23	1:A:12:LEU:H	0.69	1.47	9	5
1:A:7:LEU:HD13	1:A:8:TYR:H	0.69	1.46	6	5
1:A:8:TYR:O	1:A:11:TRP:HB3	0.68	1.87	2	9
1:A:9:ILE:HA	1:A:12:LEU:HD21	0.67	1.64	7	4
1:A:10:GLN:NE2	1:A:10:GLN:HA	0.67	2.05	3	2
1:A:6:ARG:HD3	1:A:7:LEU:N	0.65	2.05	3	3
1:A:10:GLN:HA	1:A:13:LYS:CG	0.64	2.23	2	3
1:A:8:TYR:CD2	1:A:24:PRO:HD2	0.63	2.27	9	7
1:A:10:GLN:HA	1:A:13:LYS:HG2	0.63	1.70	1	3
1:A:10:GLN:HE21	1:A:11:TRP:N	0.63	1.91	2	2
1:A:6:ARG:O	1:A:10:GLN:HG2	0.62	1.94	8	4
1:A:10:GLN:HE21	1:A:10:GLN:HA	0.61	1.55	6	1
1:A:11:TRP:HE3	1:A:12:LEU:HD23	0.61	1.55	9	4
1:A:10:GLN:NE2	1:A:11:TRP:N	0.61	2.48	1	2
1:A:7:LEU:N	1:A:7:LEU:CD2	0.59	2.65	8	1
1:A:10:GLN:HA	1:A:10:GLN:HE21	0.58	1.59	10	1
1:A:6:ARG:HD3	1:A:7:LEU:H	0.58	1.59	4	2
1:A:8:TYR:CD1	1:A:8:TYR:C	0.57	2.83	6	8
1:A:7:LEU:HD22	1:A:7:LEU:C	0.56	2.26	9	6
1:A:7:LEU:CD2	1:A:7:LEU:H	0.56	2.14	8	1
1:A:6:ARG:HA	1:A:9:ILE:HD12	0.56	1.77	3	2
1:A:10:GLN:HA	1:A:10:GLN:NE2	0.56	2.16	6	1
1:A:11:TRP:CE3	1:A:12:LEU:HD23	0.55	2.36	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:C	1:A:13:LYS:HG2	0.55	2.26	1	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.55	2.16	8	1
1:A:11:TRP:CZ3	1:A:12:LEU:HD23	0.55	2.37	6	3
1:A:11:TRP:CE3	1:A:12:LEU:HB2	0.54	2.38	1	2
1:A:10:GLN:HA	1:A:13:LYS:HG3	0.53	1.80	7	2
1:A:10:GLN:CA	1:A:13:LYS:HG2	0.53	2.32	1	2
1:A:9:ILE:O	1:A:12:LEU:HB2	0.52	2.05	4	2
1:A:10:GLN:NE2	1:A:10:GLN:CA	0.52	2.73	6	2
1:A:11:TRP:HE1	1:A:21:ARG:C	0.52	2.13	9	8
1:A:11:TRP:CE3	1:A:12:LEU:N	0.51	2.79	8	1
1:A:11:TRP:CZ3	1:A:12:LEU:CD2	0.51	2.94	4	3
1:A:7:LEU:C	1:A:10:GLN:HG3	0.51	2.31	2	2
1:A:6:ARG:HB2	1:A:7:LEU:CD2	0.50	2.36	8	1
1:A:11:TRP:O	1:A:14:GLN:HG3	0.50	2.07	3	3
1:A:10:GLN:HA	1:A:13:LYS:CD	0.50	2.37	1	1
1:A:12:LEU:HD23	1:A:12:LEU:N	0.50	2.22	9	3
1:A:11:TRP:CH2	1:A:17:PRO:CD	0.49	2.91	4	1
1:A:11:TRP:CH2	1:A:23:PRO:HB3	0.49	2.43	4	1
1:A:11:TRP:CD1	1:A:21:ARG:HB3	0.49	2.43	9	2
1:A:9:ILE:HA	1:A:12:LEU:CD2	0.49	2.38	9	2
1:A:9:ILE:O	1:A:13:LYS:HE3	0.48	2.07	2	1
1:A:11:TRP:CH2	1:A:17:PRO:HG3	0.48	2.44	7	8
1:A:10:GLN:HE21	1:A:13:LYS:HG3	0.48	1.67	7	2
1:A:13:LYS:N	1:A:13:LYS:HE2	0.48	2.23	6	1
1:A:15:GLY:O	1:A:18:SER:HB3	0.48	2.07	4	5
1:A:6:ARG:CZ	1:A:9:ILE:HD12	0.48	2.39	9	1
1:A:8:TYR:O	1:A:12:LEU:HD23	0.47	2.09	10	3
1:A:11:TRP:CE3	1:A:12:LEU:CD2	0.47	2.98	9	3
1:A:6:ARG:HD3	1:A:7:LEU:HB3	0.47	1.86	1	6
1:A:7:LEU:HD22	1:A:7:LEU:O	0.47	2.10	2	2
1:A:10:GLN:NE2	1:A:13:LYS:HG3	0.47	2.24	10	2
1:A:9:ILE:O	1:A:12:LEU:HG	0.46	2.10	7	2
1:A:7:LEU:HA	1:A:10:GLN:HG2	0.46	1.86	2	2
1:A:9:ILE:HG22	1:A:13:LYS:CE	0.45	2.41	1	1
1:A:11:TRP:CZ3	1:A:17:PRO:HD3	0.45	2.47	1	1
1:A:7:LEU:CD1	1:A:7:LEU:H	0.45	2.25	1	4
1:A:9:ILE:HA	1:A:12:LEU:HD23	0.45	1.88	1	1
1:A:10:GLN:O	1:A:14:GLN:HG3	0.44	2.12	4	1
1:A:11:TRP:CE2	1:A:17:PRO:HD3	0.44	2.43	4	1
1:A:15:GLY:O	1:A:18:SER:HB2	0.43	2.13	9	1
1:A:6:ARG:CD	1:A:6:ARG:N	0.43	2.81	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:O	1:A:13:LYS:N	0.43	2.47	8	1
1:A:7:LEU:HD13	1:A:7:LEU:C	0.42	2.40	1	3
1:A:11:TRP:CE3	1:A:12:LEU:CB	0.42	3.02	1	1
1:A:15:GLY:O	1:A:16:GLY:C	0.42	2.62	10	1
1:A:7:LEU:HA	1:A:10:GLN:CG	0.42	2.45	1	1
1:A:6:ARG:N	1:A:6:ARG:HD2	0.42	2.30	6	1
1:A:6:ARG:CD	1:A:7:LEU:H	0.41	2.29	5	1
1:A:23:PRO:HA	1:A:24:PRO:HD3	0.41	1.81	6	1
1:A:11:TRP:CE2	1:A:16:GLY:HA3	0.41	2.50	2	1
1:A:6:ARG:HB2	1:A:7:LEU:HD22	0.41	1.92	8	1
1:A:8:TYR:CE1	1:A:12:LEU:HD22	0.40	2.51	10	1
1:A:19:SER:OG	1:A:21:ARG:HD3	0.40	2.16	9	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	19/25 (76%)	16±1 (83±5%)	1±1 (6±5%)	2±1 (11±4%)	1	9
All	All	190/250 (76%)	158 (83%)	12 (6%)	20 (11%)	1	9

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	9
1	A	18	SER	9
1	A	24	PRO	1
1	A	17	PRO	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	16/21 (76%)	12±2 (76±9%)	4±2 (24±9%)	2	26
All	All	160/210 (76%)	121 (76%)	39 (24%)	2	26

All 8 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	6	ARG	9
1	A	7	LEU	9
1	A	12	LEU	6
1	A	10	GLN	5
1	A	14	GLN	5
1	A	13	LYS	2
1	A	8	TYR	2
1	A	21	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_ShiftList_1*

7.1.1 Bookkeeping

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

Total number of shifts	168
Number of shifts mapped to atoms	168
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 142 atoms were assigned a chemical shift out of a possible 267. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	37/90 (41%)	37/37 (100%)	0/38 (0%)	0/15 (0%)
Sidechain	95/156 (61%)	95/101 (94%)	0/46 (0%)	0/9 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	142/267 (53%)	142/148 (96%)	0/94 (0%)	0/25 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 167 atoms were assigned a chemical shift out of a possible 335. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	46/120 (38%)	46/49 (94%)	0/50 (0%)	0/21 (0%)
Sidechain	111/194 (57%)	111/125 (89%)	0/60 (0%)	0/9 (0%)
Aromatic	10/21 (48%)	10/10 (100%)	0/10 (0%)	0/1 (0%)
Overall	167/335 (50%)	167/184 (91%)	0/120 (0%)	0/31 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

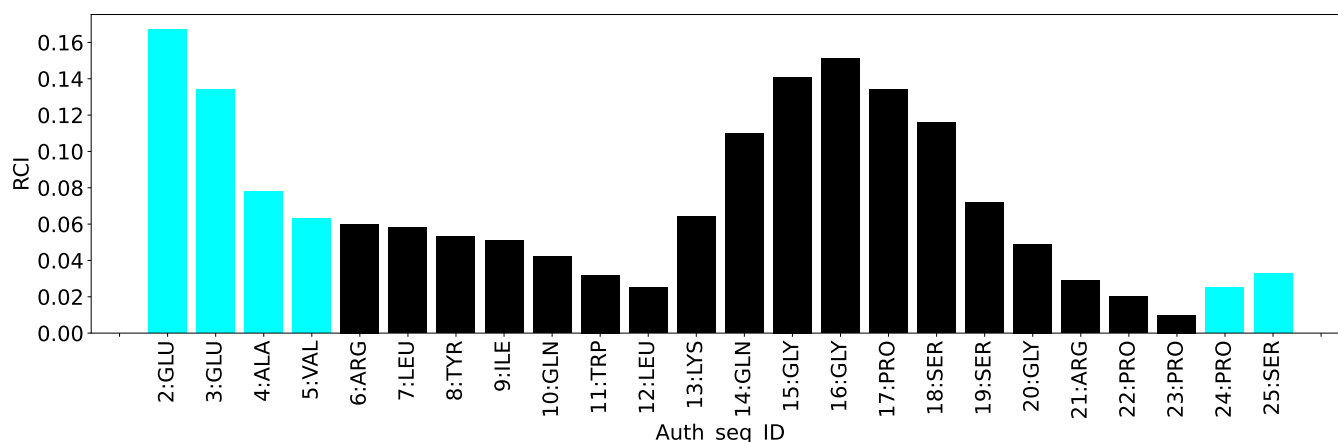
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	GLY	HA2	1.14	2.15 – 5.77	-7.8
1	A	23	PRO	HA	2.71	2.78 – 6.00	-5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

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	1707
Intra-residue ($ i-j =0$)	924
Sequential ($ i-j =1$)	414
Medium range ($ i-j >1$ and $ i-j <5$)	225
Long range ($ i-j \geq 5$)	144
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	68.3
Number of long range restraints per residue ¹	5.8

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)	84.7	0.2
0.2-0.5 (Medium)	161.5	0.5
>0.5 (Large)	185.0	4.93

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

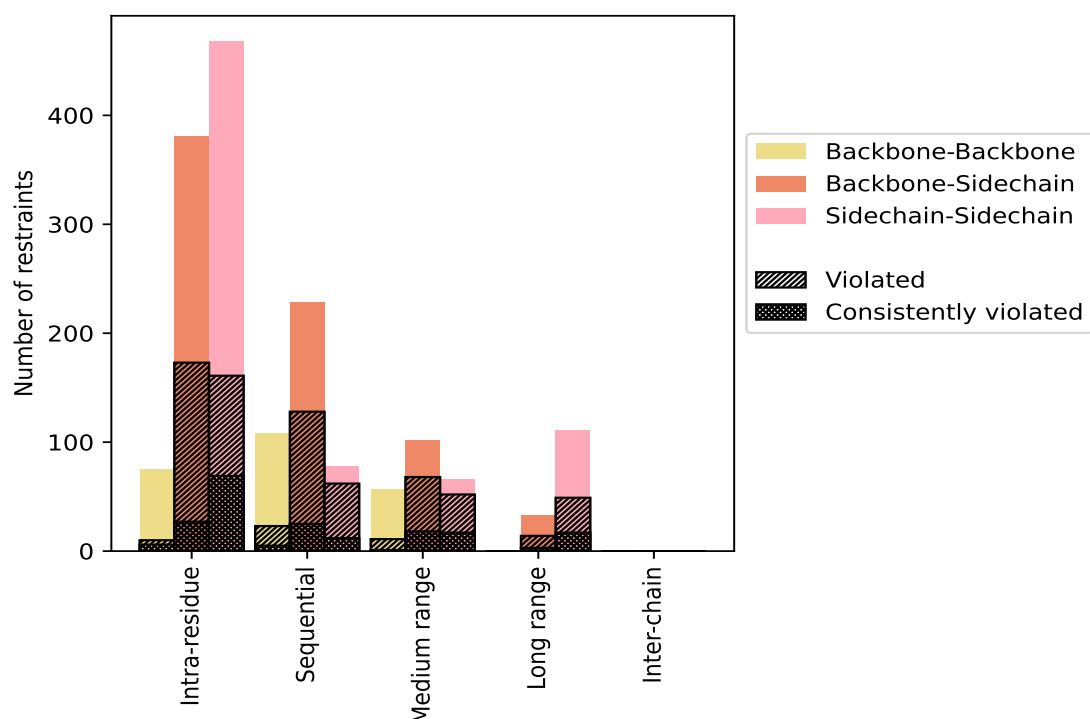
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	924	54.1	344	37.2	20.2	102	11.0	6.0
Backbone-Backbone	75	4.4	10	13.3	0.6	6	8.0	0.4
Backbone-Sidechain	381	22.3	173	45.4	10.1	27	7.1	1.6
Sidechain-Sidechain	468	27.4	161	34.4	9.4	69	14.7	4.0
Sequential (i-j =1)	414	24.3	213	51.4	12.5	42	10.1	2.5
Backbone-Backbone	108	6.3	23	21.3	1.3	5	4.6	0.3
Backbone-Sidechain	228	13.4	128	56.1	7.5	25	11.0	1.5
Sidechain-Sidechain	78	4.6	62	79.5	3.6	12	15.4	0.7
Medium range (i-j >1 & i-j <5)	225	13.2	131	58.2	7.7	36	16.0	2.1
Backbone-Backbone	57	3.3	11	19.3	0.6	1	1.8	0.1
Backbone-Sidechain	102	6.0	68	66.7	4.0	18	17.6	1.1
Sidechain-Sidechain	66	3.9	52	78.8	3.0	17	25.8	1.0
Long range (i-j ≥5)	144	8.4	63	43.8	3.7	20	13.9	1.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	33	1.9	14	42.4	0.8	3	9.1	0.2
Sidechain-Sidechain	111	6.5	49	44.1	2.9	17	15.3	1.0
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1707	100.0	751	44.0	44.0	200	11.7	11.7
Backbone-Backbone	240	14.1	44	18.3	2.6	12	5.0	0.7
Backbone-Sidechain	744	43.6	383	51.5	22.4	73	9.8	4.3
Sidechain-Sidechain	723	42.4	324	44.8	19.0	115	15.9	6.7

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

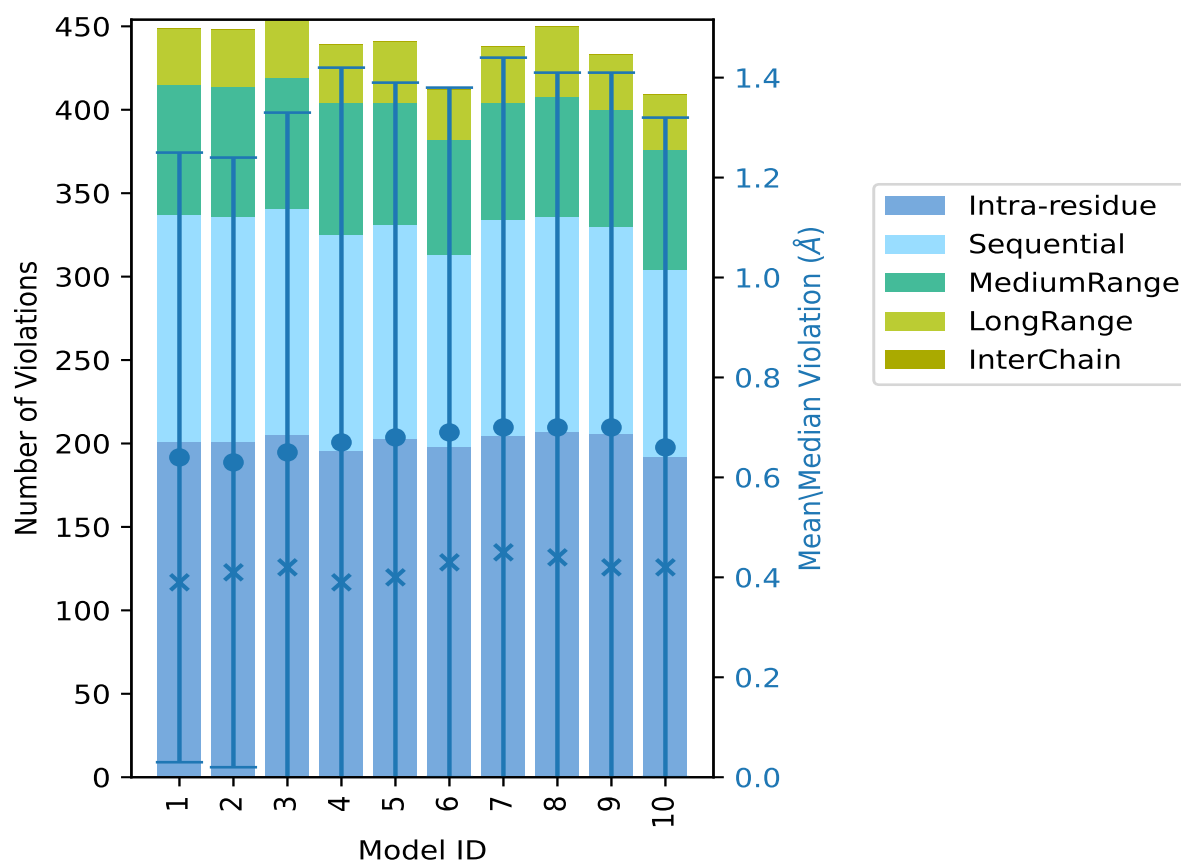
9.2 Distance violation statistics for each model [i](#)

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	201	136	78	34	0	449	0.64	3.77	0.61	0.39
2	201	135	78	34	0	448	0.63	4.27	0.61	0.41
3	205	136	78	35	0	454	0.65	4.68	0.68	0.42
4	196	129	79	35	0	439	0.67	4.52	0.75	0.39
5	203	128	73	37	0	441	0.68	4.46	0.71	0.4
6	198	115	69	30	0	412	0.69	4.65	0.69	0.43
7	205	129	70	34	0	438	0.7	4.2	0.74	0.45
8	207	129	72	42	0	450	0.7	3.93	0.71	0.44
9	206	124	70	33	0	433	0.7	4.93	0.71	0.42
10	192	112	72	33	0	409	0.66	4.61	0.66	0.42

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, 956(IR:580, SQ:201, MR:94, LR:81, 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	%
72	38	20	25	0	155	1	10.0
28	16	16	0	0	60	2	20.0
19	14	12	2	0	47	3	30.0

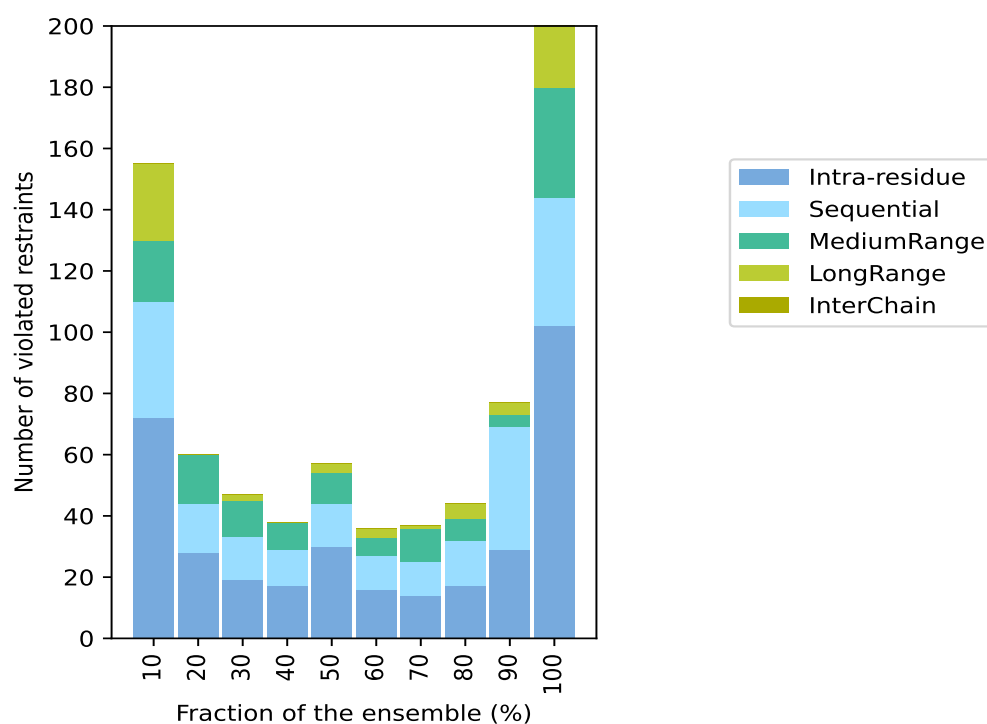
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
17	12	9	0	0	38	4	40.0
30	14	10	3	0	57	5	50.0
16	11	6	3	0	36	6	60.0
14	11	11	1	0	37	7	70.0
17	15	7	5	0	44	8	80.0
29	40	4	4	0	77	9	90.0
102	42	36	20	0	200	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

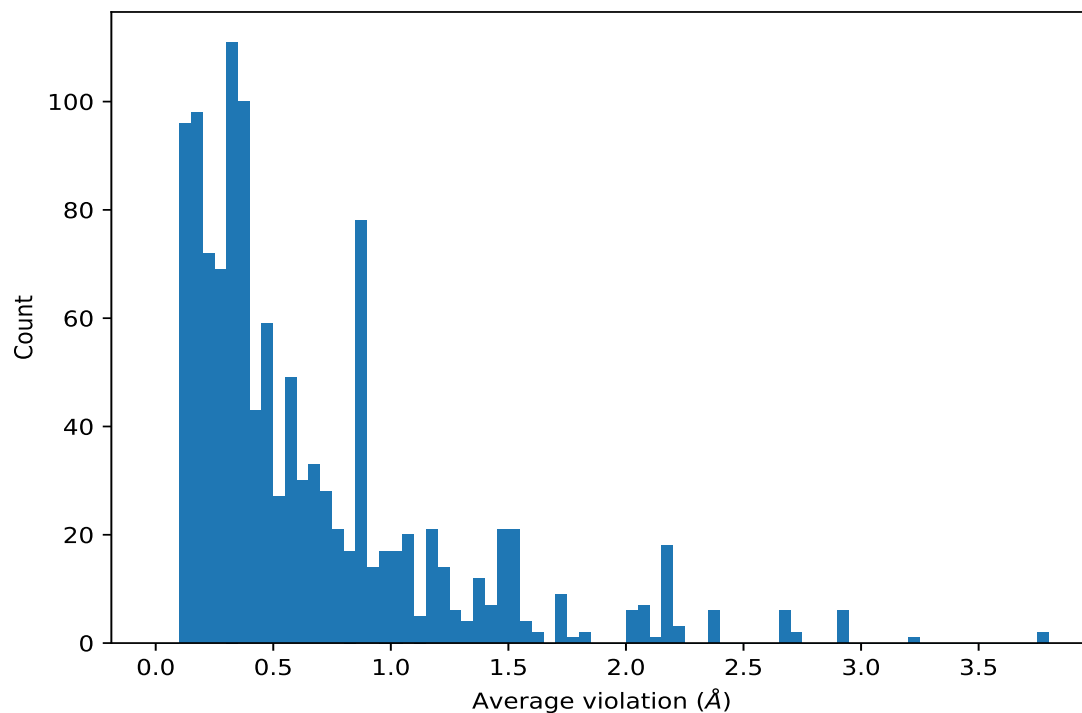


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



9.4.2 Table: Most violated distance restraints [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)
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	3.75	0.99	4.05
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	3.75	0.99	4.05
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	3.24	0.99	3.54
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.72	0.39	2.82
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.72	0.39	2.82
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	10	2.67	1.29	3.1
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	2.35	0.98	2.58
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	2.35	0.98	2.58
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	2.18	0.64	2.32
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	2.18	0.64	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	2.18	0.64	2.32
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	2.18	0.64	2.32
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	2.18	0.64	2.32
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	2.18	0.64	2.32
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	2.18	0.64	2.32
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	10	2.17	0.61	2.58
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	10	2.17	0.61	2.58
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	10	2.17	0.61	2.58
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	10	2.14	0.33	2.26
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.07	0.39	2.17
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	10	2.01	1.33	2.17
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.8	0.1	1.78
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.8	0.1	1.78
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	1.75	0.98	1.98
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.71	0.59	1.54
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	10	1.61	0.56	1.61
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	10	1.61	0.56	1.61
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	10	1.55	0.47	1.7
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	10	1.55	0.47	1.7
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	1.53	0.64	1.67
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	1.53	0.64	1.67
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	1.53	0.64	1.67
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	1.53	0.64	1.67
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	1.53	0.64	1.67
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	1.53	0.64	1.67
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	1.52	0.38	1.35
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	1.52	0.38	1.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	1.52	0.38	1.35
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	1.52	0.38	1.35
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	10	1.47	0.63	1.16
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	10	1.45	1.16	1.45
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	10	1.45	1.16	1.45
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	10	1.45	1.16	1.45
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	10	1.45	1.16	1.45
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	10	1.45	1.16	1.45
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	10	1.45	1.16	1.45
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	10	1.44	0.08	1.44
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	10	1.44	0.08	1.44
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	10	1.44	0.08	1.44
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	10	1.44	0.08	1.44
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	1.41	0.43	1.55
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	1.41	0.43	1.55
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	10	1.34	0.19	1.42
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	10	1.34	0.19	1.42
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	10	1.34	0.19	1.42
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	1.2	0.07	1.22
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	1.2	0.07	1.22
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.19	0.32	1.31
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.19	0.32	1.31
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.17	0.1	1.14
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	1.15	0.13	1.18
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	1.11	0.15	1.08
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	10	1.11	0.15	1.08
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.1	0.59	0.93
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.1	0.59	0.93
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.1	0.59	0.93
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	10	1.09	0.96	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	10	1.09	0.96	0.86
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	10	1.09	0.96	0.86
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	10	1.09	0.96	0.86
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	10	1.06	0.47	1.27
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	10	1.03	0.55	0.88
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	10	1.02	0.37	1.07
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	10	1.0	0.08	1.03
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	10	1.0	0.08	1.03
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	1.0	0.22	1.08
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	0.96	0.18	1.02
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	0.96	0.18	1.02
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.95	0.08	1.0
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.95	0.08	1.0
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.95	0.03	0.96
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.95	0.03	0.96
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.95	0.03	0.96
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.95	0.03	0.96
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.95	0.03	0.96
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.95	0.03	0.96
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.95	0.03	0.96
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.95	0.03	0.96
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.95	0.05	0.96
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.95	0.05	0.96
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.89	0.9	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.89	0.9	0.6
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.89	0.9	0.6
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	10	0.88	0.26	0.98
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	10	0.88	0.26	0.98
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	10	0.88	0.26	0.98
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	10	0.86	0.08	0.86
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	10	0.86	0.08	0.86
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.86	0.02	0.86
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	0.85	0.09	0.86
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	0.85	0.09	0.86
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	0.85	0.09	0.86
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	0.85	0.09	0.86
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	10	0.84	0.04	0.84
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.84	0.01	0.84
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.82	0.02	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.8	0.64	0.72
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.8	0.64	0.72
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.79	0.01	0.79
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	10	0.79	0.31	0.82
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	10	0.79	0.31	0.82
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	10	0.77	0.35	0.74
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	10	0.77	0.35	0.74
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.75	0.01	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.75	0.01	0.75
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	10	0.75	0.2	0.78
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.75	0.14	0.8
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.74	0.14	0.77
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	10	0.71	0.23	0.68
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	10	0.71	0.23	0.68
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.71	0.02	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.71	0.02	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.71	0.02	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.71	0.02	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.71	0.02	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.71	0.02	0.71
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.69	0.21	0.7
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.69	0.21	0.7
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	10	0.68	0.09	0.66
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	10	0.68	0.09	0.66
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	0.68	0.09	0.66
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	0.68	0.09	0.66
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	10	0.66	0.26	0.68
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	10	0.66	0.26	0.68
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	10	0.66	0.24	0.69
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.65	0.0	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.65	0.0	0.65
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	10	0.65	0.24	0.56
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.62	0.0	0.62
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.62	0.06	0.61
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	10	0.61	0.82	0.38
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	10	0.61	0.82	0.38
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	10	0.61	0.82	0.38
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	10	0.61	0.82	0.38
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	10	0.61	0.82	0.38
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	10	0.61	0.82	0.38
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.61	0.06	0.62
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.6	0.06	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.6	0.05	0.61
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.59	0.01	0.59
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	10	0.58	0.04	0.57
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	10	0.58	0.04	0.57
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.58	0.2	0.59
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.58	0.2	0.59
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.58	0.2	0.59
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	10	0.57	0.41	0.38
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	10	0.57	0.41	0.38
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.54	0.24	0.62
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.53	0.17	0.59
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.53	0.17	0.59
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	10	0.52	0.3	0.58
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	10	0.52	0.08	0.51
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.52	0.08	0.51
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.51	0.08	0.52
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.51	0.08	0.52
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.49	0.03	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.49	0.03	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	0.49	0.03	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.49	0.03	0.48
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.49	0.04	0.48
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	10	0.49	0.21	0.41
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	10	0.49	0.21	0.41
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	10	0.48	0.52	0.32
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	10	0.48	0.52	0.32
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	10	0.48	0.52	0.32
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	10	0.48	0.52	0.32
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	10	0.48	0.52	0.32
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	10	0.48	0.52	0.32
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	10	0.48	0.06	0.46
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	10	0.48	0.06	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.46	0.0	0.46
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.45	0.03	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.45	0.03	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.45	0.03	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.45	0.03	0.44
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	10	0.44	0.29	0.32
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.42	0.01	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.42	0.01	0.42
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.41	0.13	0.46
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.4	0.08	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	10	0.39	0.09	0.44
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	10	0.39	0.09	0.44
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	10	0.39	0.22	0.32
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	10	0.39	0.22	0.32
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.38	0.05	0.38
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.38	0.05	0.38
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.38	0.08	0.38
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.38	0.08	0.38
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	10	0.38	0.01	0.38
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.37	0.0	0.37
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	10	0.37	0.12	0.34
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.37	0.0	0.37
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	10	0.36	0.04	0.36
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.36	0.01	0.36
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	0.36	0.06	0.38
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.36	0.02	0.36
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.36	0.02	0.36
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.35	0.08	0.4
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.35	0.11	0.34
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.35	0.0	0.35
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.34	0.08	0.32
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.34	0.08	0.32
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.34	0.01	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.34	0.01	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.34	0.01	0.34
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.33	0.06	0.31
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.33	0.06	0.31
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.33	0.06	0.35
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.32	0.06	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.32	0.06	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.32	0.06	0.36
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	0.32	0.05	0.33
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.32	0.03	0.31
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.32	0.03	0.32
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.32	0.03	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.32	0.03	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.32	0.03	0.32
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.32	0.12	0.3
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.31	0.03	0.31
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.31	0.03	0.31
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.31	0.03	0.31
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.3	0.05	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.3	0.01	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.3	0.01	0.3
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	10	0.29	0.02	0.3
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	10	0.29	0.02	0.3
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.29	0.01	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.29	0.01	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.29	0.01	0.29
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.28	0.11	0.3
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.28	0.11	0.3
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.28	0.11	0.3
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.28	0.11	0.3
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.28	0.18	0.22
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.28	0.02	0.28
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.28	0.02	0.28
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.28	0.02	0.28
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.27	0.0	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.27	0.03	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.27	0.03	0.27
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	10	0.24	0.01	0.24
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.24	0.03	0.24
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.24	0.03	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.24	0.0	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.24	0.0	0.24
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	10	0.23	0.01	0.23
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.23	0.01	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.23	0.0	0.23
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.23	0.02	0.24
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	10	0.23	0.05	0.23
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.22	0.04	0.23
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.22	0.04	0.23
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	10	0.22	0.17	0.14
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.21	0.02	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.21	0.02	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.21	0.02	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.21	0.02	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.21	0.02	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.21	0.02	0.21
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.21	0.01	0.2
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	10	0.2	0.01	0.21
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.2	0.04	0.18
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.2	0.01	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2	0.04	0.21
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2	0.04	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2	0.04	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2	0.04	0.21
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	10	0.19	0.01	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.18	0.02	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.18	0.02	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.18	0.02	0.19
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	10	0.18	0.01	0.18
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.18	0.01	0.18
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	10	0.17	0.02	0.18
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	10	0.17	0.02	0.18
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.16	0.0	0.16
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.16	0.06	0.14
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.16	0.06	0.14
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.16	0.06	0.14
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.16	0.06	0.14
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.16	0.01	0.16
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	10	0.15	0.05	0.14
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	10	0.15	0.04	0.15
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	10	0.15	0.04	0.15
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	10	0.15	0.04	0.15
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	10	0.15	0.04	0.15
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.15	0.02	0.15
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.15	0.02	0.15
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.15	0.02	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.13	0.02	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.13	0.02	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.13	0.02	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.13	0.02	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.13	0.02	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.13	0.02	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.13	0.0	0.13
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.12	0.01	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.11	0.01	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.11	0.01	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.11	0.01	0.11
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	9	2.91	0.52	3.22
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	9	2.91	0.52	3.22
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	9	2.91	0.52	3.22
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	9	2.91	0.52	3.22
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	9	2.91	0.52	3.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	9	2.91	0.52	3.22
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	9	2.36	0.98	2.77
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	9	2.36	0.98	2.77
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	9	2.36	0.98	2.77
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	9	2.36	0.98	2.77
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	9	2.24	1.15	2.5
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	9	2.24	1.15	2.5
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	9	2.24	1.15	2.5
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	2.06	1.47	1.37
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	2.06	1.47	1.37
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	2.06	1.47	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	2.06	1.47	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	2.06	1.47	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	2.06	1.47	1.37
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	1.5	1.47	0.81
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	1.5	1.47	0.81
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	1.5	1.47	0.81
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	1.49	0.03	1.5
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	1.49	0.03	1.5
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	1.49	0.03	1.5
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	9	1.43	0.21	1.5
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	9	1.38	0.94	1.98
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	9	1.38	0.94	1.98
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	9	1.38	0.94	1.98
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	9	1.38	0.94	1.98
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	9	1.23	0.22	1.22
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.23	0.2	1.29
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.23	0.2	1.29
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	9	1.19	0.35	1.28
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	9	1.17	0.72	1.42
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	9	1.17	0.72	1.42
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	9	1.08	0.07	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	9	1.08	0.07	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	9	1.08	0.07	1.11
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	9	1.06	0.02	1.06
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	1.05	0.02	1.05
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	1.05	0.02	1.05
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	9	1.03	0.33	1.13
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	1.01	0.02	1.0
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	1.01	0.02	1.0
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	9	1.0	0.12	1.01
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	9	0.94	0.55	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	9	0.94	0.55	0.54
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	9	0.94	0.55	0.54
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	9	0.94	0.55	0.54
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	9	0.94	0.55	0.54
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	9	0.94	0.55	0.54
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	0.94	0.15	0.97
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	9	0.9	0.27	0.88
(1,284)	1:18:A:SER:H	1:19:A:SER:H	9	0.88	0.06	0.87
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	9	0.84	0.25	0.97
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	9	0.84	0.25	0.97
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	9	0.84	0.25	0.97
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	9	0.84	0.25	0.97
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	0.82	0.1	0.81
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	0.77	0.49	0.48
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	9	0.77	0.49	0.48
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.77	0.49	0.48
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	9	0.77	0.49	0.48
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	9	0.75	0.22	0.75
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	9	0.73	0.05	0.75
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.68	0.16	0.71
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	9	0.67	0.23	0.66
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.66	0.09	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	9	0.65	0.18	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	9	0.65	0.18	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	9	0.65	0.18	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	9	0.65	0.18	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	9	0.65	0.18	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	9	0.65	0.18	0.69
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.6	0.14	0.64
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.57	0.02	0.57
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.57	0.02	0.57
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.57	0.15	0.51
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.57	0.15	0.51
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	9	0.57	0.5	0.33
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	9	0.57	0.5	0.33
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	9	0.57	0.5	0.33
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.5	0.1	0.45
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	9	0.49	0.01	0.49
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	9	0.49	0.01	0.49
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.48	0.06	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.48	0.06	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.48	0.06	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.48	0.06	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.48	0.06	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.48	0.06	0.47
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.45	0.02	0.46
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	9	0.45	0.04	0.45
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	9	0.45	0.04	0.45
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	9	0.44	0.13	0.4
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.43	0.07	0.43
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.43	0.07	0.43
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.43	0.07	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.43	0.07	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.43	0.07	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.43	0.07	0.43
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.42	0.12	0.42
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.42	0.12	0.42
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.38	0.02	0.37
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.38	0.02	0.37
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.38	0.02	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.38	0.02	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.38	0.02	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.38	0.02	0.37
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	9	0.36	0.03	0.35
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.35	0.09	0.4
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.35	0.09	0.4
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	9	0.33	0.01	0.33
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	9	0.33	0.06	0.35
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	9	0.33	0.06	0.35
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	9	0.33	0.06	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	9	0.33	0.06	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	9	0.33	0.06	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	9	0.33	0.06	0.35
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.28	0.12	0.25
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.28	0.12	0.25
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.28	0.12	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.28	0.12	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.28	0.12	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.28	0.12	0.25
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.25	0.09	0.24
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.17	0.03	0.18
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	9	0.17	0.03	0.18
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	9	0.16	0.01	0.16
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	9	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	9	0.16	0.01	0.16
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	9	0.16	0.01	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.15	0.04	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.15	0.04	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.15	0.04	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.15	0.04	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.15	0.04	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.15	0.04	0.12
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	9	0.14	0.03	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	9	0.14	0.03	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	9	0.14	0.03	0.13
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	9	0.14	0.03	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	9	0.14	0.03	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	9	0.14	0.03	0.13
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	8	1.52	0.5	1.72
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	8	1.52	0.5	1.72
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	8	1.5	0.85	1.96
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	8	1.5	0.85	1.96
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	8	1.5	0.85	1.96
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	8	1.5	0.85	1.96
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	8	1.37	0.16	1.38
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	8	1.37	0.16	1.38
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	8	1.34	0.28	1.48
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.99	0.34	1.06
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.99	0.34	1.06
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	8	0.85	0.19	0.88
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	8	0.85	0.19	0.88
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	8	0.85	0.19	0.88
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	8	0.85	0.19	0.88
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.81	0.29	0.96
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	8	0.81	0.29	0.96
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	8	0.78	0.17	0.8
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	8	0.74	0.22	0.78
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	8	0.74	0.13	0.76
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	8	0.74	0.13	0.76
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	8	0.74	0.13	0.76
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.69	0.27	0.76
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	8	0.63	0.13	0.61
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	8	0.61	0.13	0.68
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.54	0.02	0.54
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.54	0.02	0.54
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.52	0.05	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.52	0.05	0.52
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.52	0.05	0.52
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.52	0.05	0.52
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.51	0.09	0.48
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	8	0.47	0.27	0.44
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	8	0.47	0.27	0.44
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	8	0.47	0.27	0.44
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.44	0.13	0.43
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.44	0.13	0.43
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	8	0.43	0.13	0.49
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	8	0.43	0.13	0.49
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.43	0.09	0.44
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.43	0.09	0.44
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	8	0.37	0.05	0.34
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	8	0.35	0.14	0.32
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	8	0.35	0.14	0.32
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	8	0.32	0.12	0.3
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	8	0.32	0.12	0.3
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.32	0.04	0.32
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.32	0.04	0.32
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	8	0.28	0.1	0.24
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	8	0.28	0.1	0.24
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	8	0.28	0.1	0.24
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.27	0.07	0.26
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	8	0.25	0.08	0.22
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.25	0.1	0.25
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.21	0.07	0.26
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.21	0.07	0.26
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	8	0.19	0.11	0.15
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	8	0.17	0.04	0.18
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	8	0.17	0.04	0.18
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	8	0.17	0.1	0.12
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	8	0.16	0.02	0.16
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	8	0.16	0.02	0.16
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	8	0.16	0.02	0.16
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	8	0.16	0.02	0.16
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	8	0.16	0.02	0.16
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	8	0.16	0.02	0.16
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	8	0.14	0.03	0.14
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	7	2.15	0.83	2.05
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	7	2.15	0.83	2.05
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	7	2.15	0.83	2.05

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	1.35	0.13	1.33
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	1.35	0.13	1.33
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	7	1.0	0.38	1.19
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.82	0.38	0.71
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	7	0.72	0.3	0.83
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	7	0.72	0.3	0.83
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	7	0.72	0.3	0.83
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	7	0.72	0.3	0.83
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	7	0.72	0.3	0.83
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	7	0.72	0.3	0.83
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	0.71	0.13	0.69
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	7	0.68	1.07	0.25
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	7	0.68	1.07	0.25
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	7	0.68	1.07	0.25
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	7	0.68	1.07	0.25
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	7	0.68	1.07	0.25
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	7	0.68	1.07	0.25
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	0.65	0.17	0.65
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.63	0.34	0.6
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.63	0.34	0.6
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.63	0.34	0.6
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.63	0.34	0.6
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.63	0.34	0.6
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.63	0.34	0.6
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	7	0.57	0.21	0.64
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	7	0.57	0.7	0.14
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	7	0.57	0.7	0.14
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	7	0.57	0.7	0.14
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	7	0.57	0.7	0.14
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	7	0.57	0.7	0.14
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	7	0.57	0.7	0.14
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.53	0.04	0.55
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.53	0.04	0.55
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	7	0.5	0.22	0.58
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	7	0.5	0.22	0.58
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.47	0.01	0.47
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.47	0.01	0.47
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	7	0.45	0.06	0.44
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	7	0.45	0.06	0.44
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	7	0.43	0.12	0.46
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.42	0.25	0.33
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.42	0.25	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.42	0.25	0.33
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	7	0.42	0.25	0.33
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	7	0.42	0.25	0.33
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	7	0.42	0.25	0.33
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	7	0.41	0.15	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	7	0.41	0.15	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	7	0.41	0.15	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	7	0.41	0.15	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	7	0.41	0.15	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	7	0.41	0.15	0.39
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	7	0.4	0.22	0.33
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	7	0.4	0.22	0.33
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	7	0.36	0.22	0.28
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	7	0.36	0.22	0.28
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	7	0.36	0.22	0.28
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	7	0.36	0.22	0.28
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.33	0.06	0.34
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.33	0.06	0.34
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	7	0.29	0.11	0.33
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	7	0.27	0.12	0.28
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.18	0.06	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.18	0.06	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.18	0.06	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.18	0.06	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.18	0.06	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.18	0.06	0.16
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	7	0.17	0.09	0.14
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	7	0.17	0.09	0.14
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	0.16	0.06	0.11
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	0.16	0.06	0.11
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	6	1.74	0.79	1.68
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	6	1.74	0.79	1.68
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	6	1.74	0.79	1.68
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	6	1.29	0.45	1.36
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	6	1.29	0.45	1.36
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	6	1.29	0.45	1.36
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	6	1.29	0.45	1.36
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	6	1.29	0.45	1.36
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	6	1.29	0.45	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	6	1.18	0.46	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	6	1.18	0.46	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	6	1.18	0.46	1.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	6	1.18	0.46	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	6	1.18	0.46	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	6	1.18	0.46	1.36
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	6	1.16	0.47	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	6	1.16	0.47	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	6	1.16	0.47	1.33
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	6	1.09	0.3	1.03
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	6	0.92	0.36	1.02
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	6	0.92	0.36	1.02
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.9	0.3	1.02
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.8	0.07	0.78
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.8	0.07	0.78
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	6	0.78	0.1	0.82
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.72	0.33	0.9
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	6	0.62	0.23	0.62
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	6	0.59	0.33	0.48
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.44	0.17	0.44
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	6	0.4	0.35	0.25
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	6	0.38	0.01	0.38
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	6	0.37	0.24	0.29
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	6	0.37	0.24	0.29
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	6	0.37	0.24	0.29
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	6	0.37	0.24	0.29
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	6	0.37	0.24	0.29
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	6	0.37	0.24	0.29
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	6	0.35	0.18	0.31
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	6	0.35	0.18	0.31
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.34	0.35	0.2
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	6	0.34	0.35	0.2
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	6	0.32	0.15	0.29
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	6	0.32	0.15	0.29
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	6	0.31	0.04	0.31
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	6	0.31	0.04	0.31
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	6	0.27	0.06	0.29
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	6	0.27	0.06	0.29
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.26	0.19	0.18
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.26	0.19	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	6	0.25	0.17	0.18
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	6	0.25	0.17	0.18
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.19	0.04	0.2
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	6	0.18	0.05	0.16
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	6	0.18	0.05	0.16
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	6	0.18	0.05	0.16
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	6	0.18	0.05	0.16
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	6	0.18	0.05	0.16
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	6	0.18	0.05	0.16
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	6	0.16	0.07	0.12
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	6	0.16	0.07	0.12
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	6	0.16	0.07	0.12
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	6	0.16	0.07	0.12
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	6	0.14	0.03	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	6	0.13	0.02	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	6	0.13	0.02	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	6	0.13	0.02	0.14
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	5	1.56	0.16	1.66
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	5	1.56	0.16	1.66
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	5	1.53	0.22	1.46
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	5	1.53	0.22	1.46
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.94	0.02	0.94
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.94	0.02	0.94
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.94	0.02	0.94
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	5	0.87	0.55	1.28
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	5	0.87	0.55	1.28
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.85	0.11	0.88
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	5	0.68	0.24	0.8
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.59	0.09	0.63
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.59	0.09	0.63
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	5	0.56	0.79	0.16
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	5	0.56	0.79	0.16
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	5	0.56	0.79	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	5	0.56	0.79	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	5	0.56	0.79	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	5	0.56	0.79	0.16
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	5	0.55	0.13	0.49
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	5	0.55	0.12	0.52
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	5	0.55	0.12	0.52
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	5	0.55	0.12	0.52
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	5	0.47	0.21	0.42
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	5	0.47	0.21	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	5	0.47	0.21	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	5	0.47	0.21	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	5	0.47	0.21	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	5	0.47	0.21	0.42
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	5	0.46	0.11	0.45
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.38	0.21	0.48
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	5	0.37	0.1	0.33
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	5	0.37	0.1	0.33
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	5	0.37	0.1	0.33
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	5	0.37	0.1	0.34
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.34	0.02	0.34
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.34	0.02	0.34
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	5	0.33	0.25	0.17
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	5	0.31	0.03	0.3
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	5	0.31	0.03	0.3
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	5	0.3	0.09	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.3	0.05	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	5	0.3	0.05	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	5	0.3	0.05	0.29
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	5	0.28	0.02	0.28
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	5	0.28	0.02	0.28
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	5	0.27	0.24	0.17
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	5	0.27	0.24	0.17
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	5	0.27	0.24	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	5	0.27	0.24	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	5	0.27	0.24	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	5	0.27	0.24	0.17
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	5	0.26	0.18	0.15
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	5	0.26	0.04	0.25
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	5	0.26	0.04	0.25
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.26	0.01	0.26
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.26	0.01	0.26
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.23	0.01	0.23
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.23	0.01	0.23
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	5	0.21	0.05	0.23
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.21	0.05	0.18
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	0.21	0.05	0.18
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	0.21	0.05	0.18
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.21	0.05	0.18
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	0.21	0.05	0.18
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	0.21	0.05	0.18
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.2	0.08	0.17
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	5	0.2	0.08	0.19
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	5	0.2	0.08	0.19
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.2	0.08	0.17
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	5	0.2	0.08	0.19
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	5	0.2	0.08	0.19
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.19	0.1	0.13
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.19	0.1	0.13
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.19	0.1	0.13
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.19	0.1	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.19	0.1	0.13
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.19	0.1	0.13
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.18	0.06	0.2
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.18	0.06	0.2
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	5	0.14	0.02	0.14
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	0.14	0.02	0.15
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	0.14	0.02	0.15
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	0.14	0.02	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	0.14	0.02	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	0.14	0.02	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	0.14	0.02	0.15
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	5	0.13	0.01	0.13
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	0.13	0.02	0.12
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	5	0.13	0.02	0.12
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	0.13	0.02	0.12
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	5	0.13	0.02	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	5	0.12	0.01	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	5	0.12	0.01	0.12
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	5	0.11	0.01	0.11
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.1	0.0	0.1
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	4	0.89	1.15	0.28
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	4	0.89	1.15	0.28
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.82	0.28	0.86
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD3	4	0.82	0.28	0.86
(1,198)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	4	0.74	0.04	0.74
(1,517)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	0.62	0.47	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	4	0.56	0.3	0.59
(1,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.54	0.13	0.59
(1,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.54	0.13	0.59
(1,224)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.51	0.1	0.52
(2,363)	1:24:A:PRO:HA	1:25:A:SER:H	4	0.42	0.09	0.46
(4,29)	1:24:A:PRO:HA	1:25:A:SER:H	4	0.42	0.09	0.46
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.38	0.07	0.41
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.38	0.07	0.41
(1,408)	1:5:A:VAL:HG11	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,408)	1:5:A:VAL:HG12	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,408)	1:5:A:VAL:HG13	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,408)	1:5:A:VAL:HG21	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,408)	1:5:A:VAL:HG22	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,408)	1:5:A:VAL:HG23	1:9:A:ILE:H	4	0.38	0.23	0.36
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	4	0.38	0.08	0.38
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	4	0.38	0.08	0.38
(1,490)	1:6:A:ARG:HA	1:9:A:ILE:HB	4	0.35	0.25	0.23
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.33	0.21	0.28
(2,412)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,412)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,412)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,412)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,412)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,412)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.32	0.01	0.32
(4,32)	1:5:A:VAL:HG11	1:6:A:ARG:H	4	0.32	0.01	0.32
(4,32)	1:5:A:VAL:HG12	1:6:A:ARG:H	4	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,32)	1:5:A:VAL:HG13	1:6:A:ARG:H	4	0.32	0.01	0.32
(4,32)	1:5:A:VAL:HG21	1:6:A:ARG:H	4	0.32	0.01	0.32
(4,32)	1:5:A:VAL:HG22	1:6:A:ARG:H	4	0.32	0.01	0.32
(4,32)	1:5:A:VAL:HG23	1:6:A:ARG:H	4	0.32	0.01	0.32
(2,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	4	0.31	0.23	0.21
(3,186)	1:10:A:GLN:H	1:10:A:GLN:HE22	4	0.31	0.23	0.21
(1,268)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	4	0.3	0.01	0.3
(1,268)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	4	0.3	0.01	0.3
(2,47)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.29	0.11	0.24
(3,43)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.29	0.11	0.24
(2,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.28	0.04	0.27
(3,17)	1:3:A:GLU:H	1:3:A:GLU:HG2	4	0.28	0.04	0.27
(1,476)	1:13:A:LYS:HB2	1:14:A:GLN:H	4	0.24	0.09	0.22
(1,360)	1:6:A:ARG:HA	1:9:A:ILE:H	4	0.23	0.11	0.18
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE2	4	0.19	0.05	0.18
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE3	4	0.19	0.05	0.18
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE2	4	0.19	0.05	0.18
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE3	4	0.19	0.05	0.18
(2,501)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	4	0.19	0.06	0.17
(3,452)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	4	0.19	0.06	0.17
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	4	0.17	0.04	0.19
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	4	0.17	0.04	0.19
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD1	4	0.17	0.04	0.19
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD2	4	0.17	0.04	0.19
(2,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.16	0.04	0.16
(3,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.16	0.04	0.16
(2,397)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	4	0.14	0.03	0.15
(2,397)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	4	0.14	0.03	0.15
(3,367)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	4	0.14	0.03	0.15
(3,367)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	4	0.14	0.03	0.15
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	4	0.12	0.02	0.12
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	4	0.12	0.02	0.12
(1,311)	1:21:A:ARG:HB3	1:21:A:ARG:HE	3	1.24	0.59	1.61
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HG	3	1.03	0.06	1.03
(1,442)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	3	0.96	0.61	1.31
(2,457)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	3	0.76	0.58	0.66
(2,457)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	3	0.76	0.58	0.66
(3,413)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	3	0.76	0.58	0.66
(3,413)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	3	0.76	0.58	0.66
(1,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	3	0.64	0.11	0.71
(2,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.62	0.01	0.63
(3,211)	1:12:A:LEU:H	1:12:A:LEU:HB3	3	0.62	0.01	0.63
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.55	0.26	0.44
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.55	0.26	0.44
(1,194)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	3	0.52	0.3	0.67
(1,194)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	3	0.52	0.3	0.67
(1,121)	1:25:A:SER:H	1:25:A:SER:HA	3	0.49	0.0	0.49
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	3	0.47	0.06	0.46
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	3	0.47	0.06	0.46
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	3	0.47	0.06	0.46
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	3	0.47	0.06	0.46
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	3	0.47	0.06	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	3	0.47	0.06	0.46
(1,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.46	0.03	0.44
(2,483)	1:13:A:LYS:H	1:14:A:GLN:HG2	3	0.46	0.38	0.25
(3,437)	1:13:A:LYS:H	1:14:A:GLN:HG2	3	0.46	0.38	0.25
(2,479)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.42	0.06	0.39
(2,479)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.42	0.06	0.39
(3,434)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	3	0.42	0.06	0.39
(3,434)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	3	0.42	0.06	0.39
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	3	0.38	0.19	0.44
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	3	0.38	0.19	0.44
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	3	0.38	0.19	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	3	0.38	0.19	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	3	0.38	0.19	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	3	0.38	0.19	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	3	0.38	0.19	0.44
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.36	0.15	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.36	0.15	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.36	0.15	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.36	0.15	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.36	0.15	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.36	0.15	0.45
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	3	0.35	0.08	0.4
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	3	0.35	0.08	0.4
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	3	0.35	0.08	0.4
(1,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	3	0.34	0.25	0.18
(2,460)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.3	0.01	0.3
(3,416)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.3	0.01	0.3
(1,229)	1:12:A:LEU:HB2	1:12:A:LEU:HG	3	0.3	0.02	0.3
(2,507)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.28	0.11	0.34
(2,507)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.28	0.11	0.34
(3,456)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.28	0.11	0.34
(3,456)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.28	0.11	0.34
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	3	0.28	0.08	0.29
(1,462)	1:6:A:ARG:HG2	1:7:A:LEU:H	3	0.27	0.07	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB2	3	0.25	0.09	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB3	3	0.25	0.09	0.31
(2,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	3	0.23	0.1	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,235)	1:14:A:GLN:H	1:14:A:GLN:HG3	3	0.23	0.1	0.17
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB1	3	0.23	0.12	0.16
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB2	3	0.23	0.12	0.16
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB3	3	0.23	0.12	0.16
(2,560)	1:9:A:ILE:HG21	1:12:A:LEU:HG	3	0.2	0.05	0.22
(2,560)	1:9:A:ILE:HG22	1:12:A:LEU:HG	3	0.2	0.05	0.22
(2,560)	1:9:A:ILE:HG23	1:12:A:LEU:HG	3	0.2	0.05	0.22
(3,493)	1:9:A:ILE:HG21	1:12:A:LEU:HG	3	0.2	0.05	0.22
(3,493)	1:9:A:ILE:HG22	1:12:A:LEU:HG	3	0.2	0.05	0.22
(3,493)	1:9:A:ILE:HG23	1:12:A:LEU:HG	3	0.2	0.05	0.22
(1,258)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	3	0.2	0.08	0.19
(2,558)	1:4:A:ALA:HB1	1:5:A:VAL:HB	3	0.19	0.01	0.19
(2,558)	1:4:A:ALA:HB2	1:5:A:VAL:HB	3	0.19	0.01	0.19
(2,558)	1:4:A:ALA:HB3	1:5:A:VAL:HB	3	0.19	0.01	0.19
(3,492)	1:4:A:ALA:HB1	1:5:A:VAL:HB	3	0.19	0.01	0.19
(3,492)	1:4:A:ALA:HB2	1:5:A:VAL:HB	3	0.19	0.01	0.19
(3,492)	1:4:A:ALA:HB3	1:5:A:VAL:HB	3	0.19	0.01	0.19
(2,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	3	0.14	0.0	0.14
(2,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	3	0.14	0.0	0.14
(3,457)	1:14:A:GLN:HB2	1:16:A:GLY:H	3	0.14	0.0	0.14
(3,457)	1:14:A:GLN:HB3	1:16:A:GLY:H	3	0.14	0.0	0.14
(1,319)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	3	0.13	0.01	0.12
(1,180)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	3	0.12	0.01	0.12
(2,529)	1:7:A:LEU:HA	1:10:A:GLN:H	3	0.12	0.01	0.11
(3,472)	1:7:A:LEU:HA	1:10:A:GLN:H	3	0.12	0.01	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	3	0.11	0.0	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	3	0.11	0.0	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	3	0.11	0.0	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD11	3	0.11	0.0	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD12	3	0.11	0.0	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD13	3	0.11	0.0	0.11
(1,91)	1:6:A:ARG:H	1:7:A:LEU:HB3	3	0.1	0.0	0.1
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	1.37	0.04	1.37
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	1.37	0.04	1.37
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	1.37	0.04	1.37
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	1.37	0.04	1.37
(2,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	2	1.24	0.13	1.24
(3,487)	1:7:A:LEU:HA	1:10:A:GLN:HG3	2	1.24	0.13	1.24
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	1.2	0.17	1.2
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	1.2	0.17	1.2
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	1.2	0.17	1.2
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	1.2	0.17	1.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	1.2	0.17	1.2
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	1.2	0.17	1.2
(1,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	2	1.16	0.1	1.16
(1,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	2	1.16	0.1	1.16
(1,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	2	1.16	0.1	1.16
(2,132)	1:18:A:SER:HB3	1:19:A:SER:HG	2	1.15	0.1	1.15
(3,118)	1:18:A:SER:HB3	1:19:A:SER:HG	2	1.15	0.1	1.15
(1,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	1.02	0.01	1.02
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	2	0.88	0.16	0.88
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	2	0.88	0.16	0.88
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	2	0.88	0.16	0.88
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	2	0.88	0.16	0.88
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	2	0.88	0.16	0.88
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	2	0.88	0.16	0.88
(1,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	2	0.76	0.02	0.76
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	2	0.72	0.3	0.72
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	2	0.72	0.3	0.72
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.72	0.3	0.72
(2,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	2	0.7	0.04	0.7
(3,50)	1:5:A:VAL:H	1:6:A:ARG:HG2	2	0.7	0.04	0.7
(1,44)	1:6:A:ARG:HA	1:6:A:ARG:HG3	2	0.66	0.2	0.66
(2,224)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.66	0.34	0.66
(3,200)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.66	0.34	0.66
(1,254)	1:14:A:GLN:HA	1:14:A:GLN:HE21	2	0.57	0.29	0.57
(1,57)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	2	0.52	0.05	0.52
(1,299)	1:21:A:ARG:HA	1:21:A:ARG:HG3	2	0.52	0.3	0.52
(1,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.48	0.26	0.48
(1,315)	1:21:A:ARG:H	1:21:A:ARG:HG3	2	0.48	0.24	0.48
(1,64)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	2	0.48	0.01	0.48
(1,521)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	2	0.45	0.21	0.45
(1,1)	1:3:A:GLU:H	1:3:A:GLU:HA	2	0.35	0.03	0.35
(1,553)	1:10:A:GLN:HA	1:13:A:LYS:HB2	2	0.35	0.03	0.35
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	2	0.32	0.16	0.32
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	2	0.32	0.16	0.32
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	2	0.32	0.16	0.32
(2,307)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.3	0.02	0.3
(3,282)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	2	0.3	0.02	0.3
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	2	0.29	0.04	0.29
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	2	0.29	0.04	0.29
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	2	0.29	0.04	0.29
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	2	0.29	0.04	0.29
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	2	0.29	0.04	0.29

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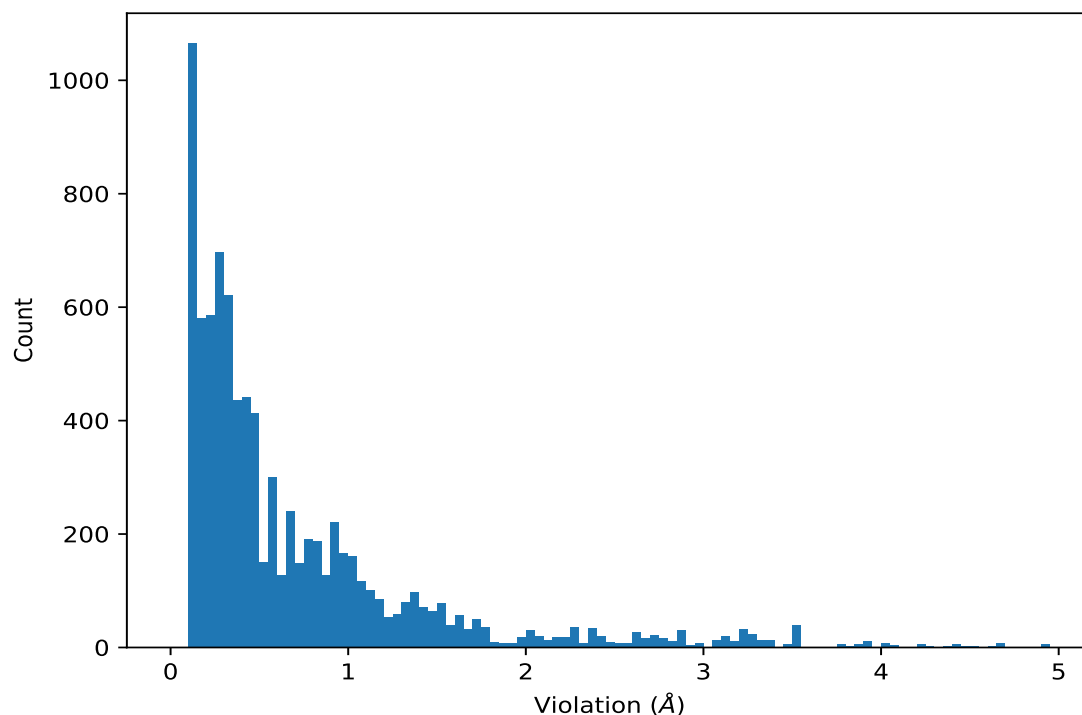
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	2	0.29	0.04	0.29
(1,460)	1:12:A:LEU:HG	1:13:A:LYS:H	2	0.28	0.01	0.28
(1,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.24	0.01	0.24
(1,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	2	0.24	0.05	0.24
(1,62)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	2	0.22	0.02	0.22
(1,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	2	0.21	0.02	0.21
(1,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	2	0.21	0.02	0.21
(2,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	2	0.21	0.1	0.21
(3,417)	1:12:A:LEU:HB2	1:13:A:LYS:H	2	0.21	0.1	0.21
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.2	0.06	0.2
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.2	0.06	0.2
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.2	0.06	0.2
(1,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.2	0.06	0.2
(2,191)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.2	0.01	0.2
(3,171)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.2	0.01	0.2
(1,402)	1:4:A:ALA:H	1:5:A:VAL:HB	2	0.18	0.03	0.18
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.18	0.02	0.18
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.18	0.02	0.18
(2,347)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.16	0.02	0.16
(3,319)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.16	0.02	0.16
(2,528)	1:8:A:TYR:HA	1:11:A:TRP:H	2	0.15	0.03	0.15
(3,471)	1:8:A:TYR:HA	1:11:A:TRP:H	2	0.15	0.03	0.15
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB1	2	0.14	0.01	0.14
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB2	2	0.14	0.01	0.14
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB3	2	0.14	0.01	0.14
(1,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	2	0.14	0.02	0.14
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB2	2	0.13	0.03	0.13
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB3	2	0.13	0.03	0.13
(2,372)	1:17:A:PRO:HD3	1:18:A:SER:H	2	0.12	0.02	0.12
(3,342)	1:17:A:PRO:HD3	1:18:A:SER:H	2	0.12	0.02	0.12
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.12	0.02	0.12
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.12	0.02	0.12
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.12	0.02	0.12
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.12	0.02	0.12
(1,395)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	2	0.11	0.01	0.11
(2,534)	1:16:A:GLY:H	1:19:A:SER:HB3	2	0.11	0.0	0.11
(3,476)	1:16:A:GLY:H	1:19:A:SER: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)
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	4.93
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	4.93
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	4.93
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	4.93
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	4.93
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	4.93
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	3	4.68
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	3	4.68
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	6	4.65
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	6	4.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	6	4.65
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	6	4.65
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	6	4.65
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	6	4.65
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	4.61
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	4.61
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	4	4.52
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	4	4.52
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	5	4.46
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	5	4.46
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	4	4.43
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	4	4.43
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	4	4.43
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	4	4.43
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	4	4.43
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	4	4.43
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	9	4.37
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	9	4.37
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	9	4.37
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	2	4.27
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	2	4.27
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	7	4.2
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	7	4.2
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	7	4.2
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	7	4.2
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	7	4.2
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	7	4.2
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	3	4.17
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	10	4.1
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	6	4.09
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	6	4.09
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	6	4.09
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	4	4.01
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	4	4.01
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	4	4.01
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	4	4.01
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	4	4.01
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	4	4.01
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	4	4.01
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	5	3.95
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	8	3.93
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	8	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	8	3.93
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	8	3.93
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	8	3.93
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	8	3.93
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	8	3.93
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	8	3.93
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	8	3.93
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	8	3.93
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	8	3.93
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	8	3.93
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	7	3.89
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	7	3.89
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	7	3.89
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	7	3.89
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	7	3.89
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	7	3.89
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	7	3.83
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	7	3.83
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	4	3.78
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	4	3.78
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	4	3.78
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	1	3.77
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	1	3.77
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	2	3.76
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	7	3.55
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	7	3.55
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	7	3.55
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	8	3.51
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	8	3.51
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	8	3.51
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	8	3.51
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	8	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	8	3.51
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	8	3.51
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	8	3.51
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	8	3.51
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	8	3.51
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	8	3.51
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	3.46
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	3.46
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	3.46
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	3.46
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	3.46
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	3.46
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	5	3.4
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	5	3.4
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	4	3.39
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	4	3.39
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	4	3.39
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	3	3.38
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	3	3.38
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	3	3.38
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	3	3.38
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	3	3.38
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	3	3.38
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	4	3.36
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	4	3.36
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	7	3.34
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	7	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	7	3.34
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	5	3.34
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	5	3.34
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	7	3.34
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	7	3.34
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	7	3.34
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	5	3.34
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	5	3.34
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	3.32
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	3.32
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	7	3.32
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	3	3.3
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	3	3.3
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	3	3.3
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	3	3.3
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	3	3.3
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	3	3.3
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	8	3.29
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	8	3.29
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	8	3.29
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	8	3.29
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	8	3.29
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	8	3.29
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	7	3.28
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	7	3.28
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	7	3.28
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	4	3.27
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	4	3.27
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	4	3.27
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	5	3.27
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	4	3.27
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	4	3.27
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	4	3.27
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	5	3.27
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	1	3.26
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	10	3.24
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	10	3.24
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	10	3.24
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	10	3.24
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	10	3.24
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	10	3.24
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	10	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	10	3.24
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	10	3.24
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	10	3.24
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	10	3.24
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	10	3.24
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	7	3.23
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	7	3.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	8	3.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	8	3.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	8	3.23
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	7	3.23
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	7	3.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	8	3.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	8	3.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	8	3.23
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	2	3.22
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	2	3.22
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	2	3.22
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	2	3.22
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	2	3.22
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	2	3.22
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	3	3.21
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	3	3.21
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	3	3.21
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	3	3.21
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	1	3.19
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	1	3.19
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	1	3.19
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	9	3.19
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	9	3.19
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	1	3.19
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	1	3.19
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	1	3.19
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	9	3.19
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	9	3.19
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	7	3.16
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	7	3.16
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	6	3.15
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	6	3.15
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	6	3.15
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	6	3.15
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	6	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	6	3.15
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	9	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	1	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	1	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	1	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	1	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	1	3.12
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	1	3.12
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	9	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	1	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	1	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	1	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	1	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	1	3.12
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	1	3.12
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	6	3.07
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	6	3.07
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	5	3.06
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	5	3.06
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	5	3.06
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	8	3.06
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	8	3.06
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	8	3.06
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	5	3.06
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	5	3.06
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	5	3.06
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	8	3.06
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	8	3.06
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	8	3.06
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	7	2.99
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	7	2.99
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	9	2.98
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	9	2.98
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	9	2.98
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	9	2.98
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	9	2.98
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	9	2.98
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.92
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.92
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	3	2.91
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	3	2.91
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	9	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	9	2.9
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	6	2.89
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	6	2.89
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	6	2.89
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	6	2.89
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	6	2.89
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	6	2.89
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	8	2.88
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	8	2.88
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	8	2.88
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	8	2.88
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	8	2.88
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	8	2.88
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	8	2.88
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	8	2.88
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	1	2.86
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	1	2.86
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	8	2.85
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	8	2.85
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	8	2.85
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	6	2.81
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	6	2.81
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	6	2.81
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	6	2.81
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	6	2.81
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	6	2.81
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	6	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	4	2.79
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	10	2.79
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	10	2.79
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	10	2.79
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	4	2.79
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	10	2.79
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	10	2.79
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	10	2.79
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	2	2.77
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	8	2.77
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	8	2.77
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	2	2.77
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	8	2.77
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	8	2.77
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	4	2.76
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	5	2.75
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	8	2.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	8	2.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	8	2.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	8	2.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	8	2.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	8	2.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	8	2.73
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	3	2.73
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	3	2.73
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	3	2.73
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	8	2.72
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	8	2.72
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	8	2.72
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	8	2.72
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	7	2.71
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	7	2.71
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	7	2.71
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	5	2.68
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	5	2.68
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	5	2.68
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	5	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	5	2.68
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	5	2.68
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	3	2.67
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	3	2.67
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	3	2.67
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	5	2.67
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	3	2.66
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	3	2.66
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	3	2.66
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	3	2.66
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	3	2.66
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	3	2.66
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	4	2.65
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	4	2.65
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	4	2.65
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	5	2.63
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	5	2.63
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	5	2.63
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	5	2.63
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	5	2.63
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	5	2.63
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	5	2.63
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	9	2.62
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	9	2.62
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	9	2.62
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	9	2.62
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	9	2.62
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	9	2.62
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	10	2.61
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	10	2.61
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	10	2.61
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	10	2.6
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	10	2.6
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	10	2.6
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	2	2.59
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	2	2.59
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	2	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	1	2.56
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	1	2.56
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	1	2.56
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	7	2.56
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	6	2.56
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	3	2.54
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	3	2.54
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	3	2.54
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	3	2.54
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	9	2.52
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	6	2.5
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	6	2.5
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	6	2.5
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	1	2.47
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	1	2.47
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	1	2.47
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	1	2.47
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	1	2.47
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	1	2.47
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	9	2.47
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	9	2.47
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	9	2.47
(1,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	8	2.43
(1,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	8	2.43
(1,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	8	2.43
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	5	2.42
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	5	2.42
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	5	2.42
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	5	2.42
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	5	2.42
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	5	2.42
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	5	2.42
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	5	2.41
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	5	2.41
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	5	2.41
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	6	2.41
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	6	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	7	2.4
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	7	2.4
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	7	2.4
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	7	2.4
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	7	2.4
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	7	2.4
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	9	2.4
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	9	2.4
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	9	2.4
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	9	2.4
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	9	2.4
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	9	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	7	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	7	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	7	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	7	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	7	2.4
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	7	2.4
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	1	2.39
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	1	2.39
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	1	2.39
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	1	2.39
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	9	2.39
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	6	2.39
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	6	2.38
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	6	2.38
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	6	2.38
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	4	2.37
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	4	2.37
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	6	2.36
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	6	2.36
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	6	2.36
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	6	2.36
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	4	2.35
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	7	2.34
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	2	2.34
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	7	2.33
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	2	2.32
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	2	2.32
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	2	2.32
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	2	2.32
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	4	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	4	2.3
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	4	2.3
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	4	2.3
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	8	2.29
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	2	2.29
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	8	2.29
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	2	2.29
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	2	2.29
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	2	2.29
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	2	2.29
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	2	2.29
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	2	2.29
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	1	2.28
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	1	2.28
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	1	2.28
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	1	2.28
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	1	2.28
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	1	2.28
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	1	2.28
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	10	2.27
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	3	2.26
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	1	2.26
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	3	2.26
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	9	2.25
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	9	2.25
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	6	2.24
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	6	2.24
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	6	2.24
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	2	2.24
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	2	2.24
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	2	2.24
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	2	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	2	2.24
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	2	2.24
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	6	2.24
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	6	2.24
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	6	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	2	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	2	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	2	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	2	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	2	2.24
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	2	2.24
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	1	2.21
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	10	2.18
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	10	2.18
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	10	2.18
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	9	2.17
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	10	2.16
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	10	2.16
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	10	2.16
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	10	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	6	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	6	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	6	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	6	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	6	2.16
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	6	2.16
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	9	2.15
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	9	2.15
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	9	2.15
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	9	2.15
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	8	2.14
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	8	2.14
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	8	2.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	8	2.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	8	2.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	8	2.14
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	4	2.14
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	2	2.12
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	5	2.1
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	5	2.1
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	5	2.1
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	5	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	5	2.1
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	5	2.1
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	8	2.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	8	2.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	8	2.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	8	2.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	8	2.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	8	2.09
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	6	2.08
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	6	2.08
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	4	2.06
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	4	2.06
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	1	2.06
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	1	2.06
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	5	2.06
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	5	2.06
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	4	2.06
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	4	2.06
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	1	2.06
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	1	2.06
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	5	2.06
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	5	2.06
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	10	2.06
(4,62)	1:3:A:GLU:HB3	1:6:A:ARG:H	6	2.05
(2,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	6	2.05
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	5	2.05
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	5	2.05
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	5	2.05
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	3	2.05
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	3	2.05
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	3	2.05
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	2	2.04
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	2	2.04
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	5	2.04
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	9	2.03
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	9	2.03
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	9	2.03
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	8	2.03
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	8	2.03
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	8	2.03
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	2	2.03
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	9	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	9	2.03
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	9	2.03
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	8	2.03
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	8	2.03
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	8	2.03
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	2	2.03
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	1	2.02
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	1	2.02
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	7	2.0
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	7	2.0
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	7	2.0
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	7	2.0
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	5	1.99
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	5	1.99
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	5	1.99
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	5	1.99
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	5	1.99
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	5	1.99
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	8	1.98
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	8	1.98
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	8	1.98
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	8	1.98
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	9	1.98
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	9	1.98
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	9	1.98
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	6	1.96
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	6	1.96
(4,67)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	6	1.96
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	6	1.96
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	6	1.96
(2,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	6	1.96
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	2	1.94
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	2	1.94
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	3	1.94
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	3	1.94
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	9	1.91
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	9	1.91
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	9	1.91
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	9	1.91
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	3	1.87
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	3	1.87
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	1	1.87
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	1.87
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	1	1.87
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	8	1.85
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	8	1.85
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	9	1.84
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	9	1.84
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	9	1.84
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	1	1.81
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	1	1.81
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	2	1.8
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.8
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	2	1.8
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.8
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	9	1.79
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	9	1.79
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	4	1.78
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	1	1.78
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	1	1.78
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	1	1.78
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	4	1.78
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	1	1.78
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	1	1.78
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	1	1.78
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	5	1.78
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	5	1.78
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	5	1.78
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	5	1.78
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	5	1.78
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	5	1.78
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	6	1.77
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	6	1.77
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	8	1.77
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	8	1.77
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	3	1.76
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	7	1.76
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	3	1.76
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	7	1.76
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	7	1.75
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	7	1.75
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	7	1.75
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	7	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	7	1.75
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	7	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	3	1.75
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	4	1.74
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	4	1.74
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	4	1.74
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	4	1.74
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	4	1.74
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	4	1.74
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	7	1.74
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	7	1.74
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	1	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	1.73
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	3	1.73
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	4	1.73
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	1	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	1.73
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	1.73
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	3	1.73
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	4	1.73
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	2	1.73
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	2	1.73
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	9	1.73
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	9	1.73
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	9	1.72
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	9	1.72
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	9	1.72
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	9	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	9	1.72
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	9	1.72
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	1	1.72
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	6	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	9	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	9	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	9	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	9	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	9	1.72
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	9	1.72
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	1	1.72
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	6	1.72
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	6	1.72
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	6	1.72
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	2	1.71
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	2	1.71
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	6	1.7
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	6	1.7
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	7	1.7
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	5	1.7
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	7	1.7
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	10	1.7
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	7	1.7
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	6	1.7
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	6	1.7
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	5	1.7
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	7	1.7
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	10	1.7
(1,311)	1:21:A:ARG:HB3	1:21:A:ARG:HE	7	1.7
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	4	1.7
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	4	1.7
(4,64)	1:2:A:GLU:HA	1:3:A:GLU:HB3	5	1.69
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	3	1.69
(2,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	5	1.69
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	3	1.69
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	5	1.69
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	1.68
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	9	1.68
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	1.68
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	9	1.68
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	5	1.68
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	5	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	2	1.68
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	2	1.68
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	3	1.68
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	3	1.68
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	4	1.66
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	4	1.66
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	1.65
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	1.65
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	2	1.65
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	2	1.65
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	2	1.65
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	2	1.65
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	2	1.65
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	2	1.65
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	5	1.64
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	5	1.64
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	8	1.64
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	1	1.64
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	1	1.64
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	1	1.64
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	1	1.64
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	1	1.64
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	1	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	9	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	9	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	9	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	9	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	9	1.64
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	9	1.64
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	9	1.63
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	9	1.63
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	9	1.63
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	9	1.63
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	9	1.63
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	9	1.63
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	6	1.63
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	6	1.63
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	6	1.63
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	6	1.61
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	6	1.61
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	6	1.61
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	6	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	6	1.61
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	6	1.61
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	8	1.61
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	1.61
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	1.61
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	1.61
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	8	1.61
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	1.61
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	1.61
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	1.61
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	6	1.61
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	6	1.61
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	6	1.61
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	6	1.61
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	6	1.61
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	6	1.61
(1,311)	1:21:A:ARG:HB3	1:21:A:ARG:HE	6	1.61
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	9	1.6
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	10	1.6
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	6	1.6
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	6	1.6
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	2	1.59
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	2	1.59
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	2	1.59
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	2	1.59
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	2	1.59
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	2	1.59
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	10	1.58
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	10	1.58
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	1.58
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	1.58
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	8	1.58
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	8	1.58
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	8	1.58
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	10	1.58
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	10	1.58
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	1.58
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	1.58
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	8	1.58
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	8	1.58
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	8	1.58
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	9	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	9	1.56
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	9	1.56
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	9	1.56
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	9	1.56
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	9	1.56
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	8	1.56
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	8	1.56
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	8	1.56
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	10	1.56
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	10	1.56
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	1.55
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	1.55
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	1.55
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	1.55
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	1.55
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	1.55
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	5	1.55
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	3	1.55
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	2	1.54
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	6	1.54
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	1.54
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	1.54
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	1.54
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	5	1.54
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	5	1.54
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	5	1.54
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	2	1.54
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	6	1.54
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	1.54
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	1.54
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	1.54
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	5	1.54
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	5	1.54
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	5	1.54
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	7	1.54
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	9	1.54
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	9	1.54
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	5	1.54
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	5	1.54
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	5	1.54
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	9	1.53
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	4	1.53
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	9	1.53
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	9	1.53
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	4	1.53
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	8	1.52
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	8	1.52
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	2	1.52
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	1.52
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	1.52
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	1.52
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	1.52
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	1.52
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	1.52
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	8	1.52
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	8	1.52
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	2	1.52
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	1.52
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	1.52
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	1.52
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	1.52
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	1.52
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	1.52
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	1	1.52
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	1	1.52
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	1	1.52
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	3	1.51
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	6	1.51
(3,413)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	8	1.51
(3,413)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	8	1.51
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	3	1.51
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	6	1.51
(2,457)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	8	1.51
(2,457)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	8	1.51
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	3	1.51
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	1.51
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	1.51
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	1.51
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	1.51
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	1.51
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	1.51
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	8	1.5
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	9	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	7	1.5
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	7	1.5
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	4	1.5
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	1.5
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	1.5
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	1.5
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	1.5
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	1.5
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	1.5
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	1.5
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	1.5
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	1.5
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	2	1.5
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	5	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	5	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	5	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	7	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	7	1.49
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	7	1.49
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	5	1.49
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	5	1.49
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	5	1.49
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	9	1.49
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	5	1.49
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	5	1.49
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	5	1.49
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	5	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	5	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	5	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	7	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	7	1.49
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	7	1.49
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	9	1.49
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	5	1.49
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	1	1.49
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	7	1.49
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	1	1.48
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	1	1.48
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	7	1.48
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	7	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	7	1.48
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	1	1.48
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	1	1.48
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	7	1.48
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	7	1.48
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	7	1.48
(1,442)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	6	1.48
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	5	1.48
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	5	1.48
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	5	1.48
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	3	1.48
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	4	1.48
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	10	1.48
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	1.47
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	1.47
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	1.47
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	1.47
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	4	1.47
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	4	1.47
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	4	1.47
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	1	1.47
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	1	1.47
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	2	1.47
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	1.47
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	1.47
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	1.47
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	1.47
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	1.47
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	1.47
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	10	1.46
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	10	1.46
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	3	1.46
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	3	1.46
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	3	1.46
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	5	1.46
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	5	1.46
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.45
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	1.45
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	2	1.45
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	2	1.45
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	2	1.45
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	8	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	10	1.45
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	4	1.44
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	4	1.44
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	4	1.44
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	4	1.44
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	6	1.44
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	2	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	4	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	4	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	4	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	4	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	4	1.44
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	4	1.44
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	3	1.43
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	3	1.43
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	3	1.43
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	3	1.43
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	1.43
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	1.43
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	1.43
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	1.43
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	3	1.43
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	3	1.43
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	3	1.43
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	3	1.43
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	1.43
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	1.43
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	1.43
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	1.43
(1,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	4	1.43
(1,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	4	1.43
(1,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	4	1.43
(1,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	8	1.43
(1,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	8	1.43
(1,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	8	1.43
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	2	1.42
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	2	1.42
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	5	1.42
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	2	1.42
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	2	1.42
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	5	1.42
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	3	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	3	1.42
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	3	1.42
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	3	1.42
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	3	1.42
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	3	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	3	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	3	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	3	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	10	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	10	1.42
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	10	1.42
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	10	1.41
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	10	1.41
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	10	1.41
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	1.41
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	1.41
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	1.41
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	1.41
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	10	1.41
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	10	1.41
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	10	1.41
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	1	1.41
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	1	1.41
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	5	1.4
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	1	1.4
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	1	1.4
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	1	1.4
(3,451)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.4
(3,451)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.4
(3,451)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.4
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	5	1.4
(2,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	1.4
(2,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	1.4
(2,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	1.4
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	1	1.4
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	1	1.4
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	1	1.4
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	9	1.4
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	9	1.4
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	9	1.4
(1,539)	1:3:A:GLU:HB3	1:6:A:ARG:H	6	1.4
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	6	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	8	1.4
(1,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	8	1.4
(1,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	8	1.4
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	7	1.4
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	7	1.4
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	9	1.4
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	6	1.39
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	6	1.39
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	2	1.39
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	1	1.39
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	1	1.39
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	1	1.39
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	2	1.39
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	2	1.39
(4,59)	1:3:A:GLU:HG3	1:7:A:LEU:H	8	1.38
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	5	1.38
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	5	1.38
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	1.38
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	1.38
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	1.38
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	1.38
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	1.38
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	1.38
(2,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	8	1.38
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	5	1.38
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	5	1.38
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	5	1.38
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	1.37
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	9	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	2	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	2	1.37
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	2	1.37
(3,487)	1:7:A:LEU:HA	1:10:A:GLN:HG3	4	1.37
(2,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	4	1.37
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	1.37
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	9	1.37
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	2	1.37
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	2	1.37
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	2	1.37
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	6	1.37
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	6	1.37
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	4	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	4	1.36
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	8	1.36
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	8	1.36
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	7	1.36
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	7	1.36
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	4	1.36
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	4	1.36
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	8	1.36
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	8	1.36
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	7	1.36
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	7	1.36
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	7	1.36
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	3	1.36
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	3	1.36
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	4	1.35
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.35
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	4	1.35
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	9	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	10	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	10	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	10	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	10	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	10	1.35
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	10	1.35
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	4	1.35
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	2	1.34
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	2	1.34
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	5	1.34
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	5	1.34
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	1.34
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.34
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	2	1.34
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	2	1.34
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	5	1.34
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	5	1.34
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	1.34
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	1.34
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	1.34
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	6	1.34
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	6	1.34
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	6	1.34
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	10	1.34
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	10	1.34
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	8	1.34
(1,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	8	1.34
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	1	1.34
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	4	1.34
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	1.33
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	1.33
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	1	1.33
(3,409)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	1	1.33
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.33
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	1.33
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	1.33
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	1	1.33
(2,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	1	1.33
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	1.33
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	7	1.33
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	7	1.33
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	7	1.33
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	9	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	1.33
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	1.33
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	2	1.32
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	2	1.32
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	1.32
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	2	1.32
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	2	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	1.32
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	7	1.32
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	7	1.32
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	7	1.32
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	8	1.31
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	9	1.31
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	4	1.31
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	4	1.31
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	4	1.31
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.31
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.31
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	8	1.31
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	9	1.31
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	1.31
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	1.31
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	4	1.31
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	4	1.31
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	4	1.31
(1,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	9	1.31
(1,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	9	1.31
(1,442)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	9	1.31
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	2	1.31
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	2	1.31
(4,58)	1:18:A:SER:HB2	1:21:A:ARG:H	6	1.3
(4,58)	1:18:A:SER:HB3	1:21:A:ARG:H	6	1.3
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	7	1.3
(2,532)	1:18:A:SER:HB2	1:21:A:ARG:H	6	1.3
(2,532)	1:18:A:SER:HB3	1:21:A:ARG:H	6	1.3
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	7	1.3
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	9	1.3
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	5	1.3
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	7	1.3
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	2	1.3
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	1.29
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	6	1.29
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	6	1.29
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	3	1.29
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	1.29
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	1.29
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	1.29
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	6	1.29
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	6	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	3	1.29
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	1.29
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	1.29
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	3	1.28
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.28
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	1.28
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	3	1.28
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	1.28
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	1.28
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	4	1.28
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	4	1.28
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	10	1.28
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	7	1.27
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	7	1.27
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	7	1.27
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	7	1.27
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	1	1.27
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	4	1.27
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	4	1.27
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	1.27
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	1.27
(1,86)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	1.27
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	7	1.27
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	7	1.27
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	7	1.26
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	9	1.26
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	10	1.26
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	10	1.26
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	10	1.26
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	7	1.26
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	9	1.26
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	10	1.26
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	10	1.26
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	10	1.26
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	10	1.26
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	10	1.26
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	5	1.26
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	9	1.26
(1,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	1	1.26
(1,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	1	1.26
(1,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	1	1.26
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	1	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	3	1.25
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	3	1.25
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	1.25
(3,118)	1:18:A:SER:HB3	1:19:A:SER:HG	1	1.25
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	3	1.25
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	3	1.25
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	1.25
(2,132)	1:18:A:SER:HB3	1:19:A:SER:HG	1	1.25
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	2	1.24
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	5	1.24
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	2	1.24
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	5	1.24
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	3	1.24
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	1.23
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	1.23
(4,63)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	1.23
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	3	1.23
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	8	1.23
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	1.23
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	1.23
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	3	1.23
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	8	1.23
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	1.23
(2,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	1.23
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	1.23
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	1	1.23
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	5	1.23
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	7	1.23
(1,313)	1:21:A:ARG:HE	1:21:A:ARG:HG3	8	1.23
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	3	1.22
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	3	1.22
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	3	1.22
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	3	1.22
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	3	1.22
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	3	1.22
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	8	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	3	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	3	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	3	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	3	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	3	1.22
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	3	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	8	1.22
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	8	1.22
(1,517)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	4	1.22
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	10	1.22
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	1	1.21
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	1	1.21
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	1	1.21
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.21
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	1	1.21
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	1	1.21
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	1	1.21
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	1.21
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	1	1.21
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	10	1.21
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	10	1.21
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	10	1.21
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	4	1.21
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	10	1.21
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	10	1.21
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	8	1.21
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	6	1.2
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	4	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	4	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	4	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	4	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	4	1.2
(4,33)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	4	1.2
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.2
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	6	1.2
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	4	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	4	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	4	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	4	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	4	1.2
(2,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	4	1.2
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	1.2
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	2	1.2
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	2	1.2
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	6	1.2
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	4	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	6	1.19
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	6	1.19
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	6	1.19
(3,389)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	8	1.19
(3,389)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	8	1.19
(3,389)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	8	1.19
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	6	1.19
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	6	1.19
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	6	1.19
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	4	1.19
(2,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	8	1.19
(2,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	8	1.19
(2,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	8	1.19
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	8	1.19
(4,57)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	8	1.18
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	4	1.18
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	4	1.18
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	4	1.18
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	4	1.18
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	4	1.18
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	4	1.18
(2,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	8	1.18
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	4	1.18
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	4	1.18
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	4	1.18
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	4	1.18
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	4	1.18
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	4	1.18
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	2	1.18
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	8	1.18
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	2	1.18
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	10	1.18
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	6	1.18
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	6	1.18
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	9	1.17
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	9	1.17
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	2	1.17
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	6	1.17
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	10	1.17
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	6	1.17
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD2	5	1.17
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD3	5	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	2	1.17
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	10	1.16
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	1	1.16
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	1	1.16
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	10	1.16
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	2	1.16
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	10	1.16
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	7	1.16
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	5	1.16
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	5	1.16
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	1	1.16
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	4	1.16
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	5	1.16
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	7	1.16
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	7	1.16
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	1.16
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	7	1.16
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	1.16
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	1.16
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	1.16
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	8	1.16
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	8	1.16
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	1.15
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.15
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	1.15
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	1.15
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	3	1.15
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	9	1.15
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	9	1.15
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	1.15
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	1.15
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	1.15
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	3	1.14
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	3	1.14
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	3	1.14
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	8	1.14
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	8	1.14
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	8	1.14
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	8	1.14
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	8	1.14
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	8	1.14
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	3	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	3	1.14
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	3	1.14
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	8	1.14
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	8	1.14
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	8	1.14
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	8	1.14
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	8	1.14
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	8	1.14
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	4	1.14
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	4	1.14
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	7	1.14
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	3	1.13
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	3	1.13
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	3	1.13
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	3	1.13
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	3	1.13
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	3	1.13
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	3	1.13
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	3	1.13
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	7	1.13
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	4	1.13
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	4	1.13
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	3	1.13
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	7	1.13
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	10	1.13
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	3	1.13
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	1	1.13
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	1	1.13
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	1	1.13
(1,48)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	1.13
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	1.12
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	1	1.12
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	7	1.12
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	7	1.12
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	7	1.12
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	7	1.12
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	7	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	7	1.12
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	1.12
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	1	1.12
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	7	1.12
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	7	1.12
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	7	1.12
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	7	1.12
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	7	1.12
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	7	1.12
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	1	1.12
(3,487)	1:7:A:LEU:HA	1:10:A:GLN:HG3	7	1.11
(2,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	7	1.11
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD21	8	1.11
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD22	8	1.11
(1,559)	1:6:A:ARG:HB2	1:7:A:LEU:HD23	8	1.11
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	7	1.11
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	8	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	3	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	3	1.11
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	3	1.11
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	5	1.1
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	5	1.1
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	5	1.1
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	5	1.1
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	1	1.1
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	7	1.1
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HG	2	1.1
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	1	1.1
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	1	1.1
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	1	1.1
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	1	1.1
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	1	1.1
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	1	1.1
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	10	1.1
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	10	1.1
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	10	1.1
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	9	1.1
(4,52)	1:11:A:TRP:H	1:12:A:LEU:HB3	3	1.09
(2,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	3	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	2	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	10	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	10	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	10	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	10	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	10	1.09
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	10	1.09
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	4	1.09
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	10	1.08
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	10	1.08
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	10	1.08
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	10	1.08
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	10	1.08
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	10	1.08
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	10	1.08
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	6	1.08
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	10	1.08
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	9	1.08
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	9	1.08
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	2	1.08
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	2	1.08
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	8	1.08
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	8	1.08
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	6	1.08
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	6	1.08
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	6	1.08
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	3	1.08
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	4	1.08
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	7	1.07
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	7	1.07
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	1	1.07
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	6	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	6	1.07
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	6	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	7	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	7	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	7	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	7	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	7	1.07
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	7	1.07
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	6	1.07
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	6	1.07
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	8	1.07
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	8	1.07
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	9	1.07
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	9	1.07
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	1	1.07
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	6	1.07
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	4	1.07
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	4	1.07
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	4	1.07
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	3	1.06
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	3	1.06
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	1.06
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	1.06
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.06
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	1.06
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	1.06
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	1.06
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	1.06
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	1.06
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	3	1.06
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	3	1.06
(1,549)	1:2:A:GLU:HA	1:3:A:GLU:HB3	5	1.06
(1,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	8	1.06
(1,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	8	1.06
(1,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	8	1.06
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	5	1.06
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	5	1.06
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	7	1.06
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	7	1.06
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	6	1.06
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	7	1.06
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	7	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	9	1.06
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	9	1.06
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	7	1.06
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	7	1.06
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	2	1.06
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	7	1.06
(4,53)	1:11:A:TRP:H	1:11:A:TRP:HD1	8	1.05
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	1.05
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	1.05
(3,118)	1:18:A:SER:HB3	1:19:A:SER:HG	9	1.05
(2,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	8	1.05
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	1.05
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	1.05
(2,132)	1:18:A:SER:HB3	1:19:A:SER:HG	9	1.05
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	3	1.05
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	5	1.05
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	5	1.05
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	5	1.05
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	8	1.05
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	8	1.05
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	10	1.05
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	10	1.05
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	5	1.05
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	7	1.05
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	10	1.05
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	5	1.05
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	5	1.05
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	5	1.05
(1,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	9	1.05
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	9	1.05
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	2	1.05
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	1	1.04
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	1	1.04
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	1	1.04
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	1	1.04
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	1	1.04
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	1	1.04
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	1.04
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	1.04
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	1	1.04
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	1	1.04
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	1	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	1	1.04
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	1.04
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	1.04
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	1.04
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	1.04
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	1	1.04
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	1	1.04
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	1	1.04
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	1	1.04
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	1	1.04
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	1	1.04
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	1	1.04
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	1	1.04
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	1	1.04
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	1	1.04
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	3	1.04
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	8	1.04
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	5	1.04
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	4	1.04
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	10	1.04
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	9	1.03
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	9	1.03
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD11	1	1.03
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD12	1	1.03
(3,490)	1:9:A:ILE:HA	1:12:A:LEU:HD13	1	1.03
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	8	1.03
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	1	1.03
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	1	1.03
(2,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	1	1.03
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	9	1.03
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	9	1.03
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	8	1.03
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HG	4	1.03
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	3	1.03
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	3	1.03
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	4	1.03
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	4	1.03
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	3	1.03
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	8	1.03
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	8	1.03
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	8	1.03
(1,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	1	1.03
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	1	1.03
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	1	1.03
(1,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	9	1.03
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	1	1.02
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	7	1.02
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	7	1.02
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	8	1.02
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	8	1.02
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	8	1.02
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	4	1.02
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	1	1.02
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	7	1.02
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	7	1.02
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	4	1.02
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	8	1.02
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	8	1.02
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	8	1.02
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	4	1.02
(1,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	9	1.02
(1,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	9	1.02
(1,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	9	1.02
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	1	1.02
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	1	1.02
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	5	1.02
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	5	1.02
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	5	1.02
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	5	1.02
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	6	1.02
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	6	1.02
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	6	1.02
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	4	1.02
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	2	1.01
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	7	1.01
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	1.01
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	1.01
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	2	1.01
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	7	1.01
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	6	1.01
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	9	1.01
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	1	1.01
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	6	1.01
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	2	1.01
(1,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	2	1.01
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	9	1.01
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	9	1.01
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	9	1.01
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	3	1.01
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	9	1.0
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	9	1.0
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	9	1.0
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	9	1.0
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	9	1.0
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	9	1.0
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	9	1.0
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	9	1.0
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	1.0
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	1.0
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	10	1.0
(3,200)	1:12:A:LEU:H	1:12:A:LEU:HG	8	1.0
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	1.0
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	1.0
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	9	1.0
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	9	1.0
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	9	1.0
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	9	1.0
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	9	1.0
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	9	1.0
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	9	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	9	1.0
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	9	1.0
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	9	1.0
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	9	1.0
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	9	1.0
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	9	1.0
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	4	1.0
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	7	1.0
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	10	1.0
(2,224)	1:12:A:LEU:H	1:12:A:LEU:HG	8	1.0
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	1.0
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	1.0
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	6	1.0
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	10	1.0
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	10	1.0
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	8	1.0
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	9	1.0
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	4	1.0
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	4	1.0
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	4	1.0
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	5	1.0
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	5	1.0
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	1	1.0
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	9	1.0
(3,444)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.99
(3,437)	1:13:A:LYS:H	1:14:A:GLN:HG2	4	0.99
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	5	0.99
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.99
(2,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.99
(2,483)	1:13:A:LYS:H	1:14:A:GLN:HG2	4	0.99
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	5	0.99
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.99
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	3	0.99
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	9	0.99
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	3	0.99
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	3	0.99
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	2	0.99
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	2	0.99
(1,284)	1:18:A:SER:H	1:19:A:SER:H	9	0.99
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	7	0.99
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	7	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	7	0.99
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	8	0.98
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	8	0.98
(4,42)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	8	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	1	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	1	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	1	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	1	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	5	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	5	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	5	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	5	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	7	0.98
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	7	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	7	0.98
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	7	0.98
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	9	0.98
(3,213)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.98
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.98
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	8	0.98
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	8	0.98
(2,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	8	0.98
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	9	0.98
(2,238)	1:13:A:LYS:H	1:13:A:LYS:HB3	2	0.98
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	1	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	1	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	1	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	1	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	5	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	5	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	5	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	5	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	7	0.98
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	7	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	7	0.98
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	7	0.98
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	10	0.98
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	6	0.98
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	6	0.98
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	9	0.98
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	9	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	5	0.98
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	5	0.98
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	5	0.98
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	7	0.98
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	7	0.98
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	7	0.98
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	1	0.98
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	1	0.98
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	2	0.98
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	2	0.98
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	2	0.98
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	5	0.98
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.97
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	1	0.97
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	1	0.97
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	1	0.97
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	2	0.97
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	2	0.97
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	2	0.97
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	6	0.97
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	6	0.97
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	3	0.97
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	3	0.97
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	3	0.97
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	3	0.97
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	6	0.97
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	6	0.97
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	6	0.97
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	6	0.97
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.97
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.97
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	1	0.97
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	1	0.97
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	1	0.97
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	2	0.97
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	2	0.97
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	2	0.97
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	6	0.97
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	6	0.97
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.97
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	3	0.97
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	3	0.97
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	3	0.97
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	6	0.97
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	6	0.97
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	6	0.97
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	6	0.97
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	5	0.97
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	10	0.97
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	8	0.97
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	6	0.97
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	6	0.97
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	6	0.97
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	6	0.97
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	6	0.97
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	6	0.97
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	6	0.97
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	6	0.97
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	9	0.97
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	9	0.97
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	7	0.97
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	1	0.97
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	1	0.97
(1,294)	1:21:A:ARG:H	1:21:A:ARG:HD2	9	0.97
(1,294)	1:21:A:ARG:H	1:21:A:ARG:HD3	9	0.97
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	5	0.97
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	5	0.97
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	5	0.97
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	5	0.97
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	9	0.97
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	9	0.97
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.97
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	9	0.97
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	7	0.97
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	1	0.97
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	1	0.96
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.96
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.96
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.96
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.96
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	1	0.96
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.96
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.96
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.96
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	1	0.96
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	2	0.96
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	6	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.96
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.96
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	2	0.96
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	2	0.96
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	2	0.96
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	2	0.96
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	2	0.96
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	2	0.96
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	2	0.96
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	2	0.96
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	3	0.96
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	3	0.96
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	6	0.96
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	9	0.96
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	3	0.96
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	4	0.95
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	4	0.95
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	4	0.95
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	4	0.95
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	9	0.95
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	9	0.95
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	9	0.95
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	9	0.95
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	4	0.95
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	4	0.95
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	4	0.95
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	4	0.95
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	9	0.95
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	9	0.95
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	9	0.95
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	9	0.95
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	9	0.95
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	9	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	4	0.95
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	8	0.95
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	8	0.95
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	9	0.95
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	9	0.95
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	9	0.95
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	9	0.95
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	9	0.95
(1,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	9	0.95
(1,438)	1:11:A:TRP:HE3	1:12:A:LEU:HG	6	0.95
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	7	0.95
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	7	0.95
(1,284)	1:18:A:SER:H	1:19:A:SER:H	8	0.95
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	4	0.95
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	4	0.95
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	4	0.95
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	4	0.95
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	10	0.95
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	10	0.95
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	2	0.94
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	2	0.94
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	2	0.94
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	2	0.94
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	8	0.94
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	8	0.94
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	8	0.94
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	8	0.94
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	5	0.94
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	5	0.94
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	2	0.94
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	2	0.94
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	2	0.94
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	2	0.94
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	8	0.94
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	8	0.94
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	8	0.94
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	8	0.94
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	8	0.94
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	8	0.94
(1,517)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	1	0.94
(1,457)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	8	0.94
(1,457)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	8	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	6	0.94
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	6	0.94
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.94
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.94
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.94
(1,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	3	0.94
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	1	0.94
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	8	0.94
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	7	0.93
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	7	0.93
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	7	0.93
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	7	0.93
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	7	0.93
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	7	0.93
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	5	0.93
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	5	0.93
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	5	0.93
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	3	0.93
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	3	0.93
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	3	0.93
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	3	0.93
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	5	0.93
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	5	0.93
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	5	0.93
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	7	0.93
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	7	0.93
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	7	0.93
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	3	0.93
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	3	0.93
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	3	0.93
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	9	0.93
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD2	6	0.93
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD3	6	0.93
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	3	0.93
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	4	0.93
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	5	0.92
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	5	0.92
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	10	0.92
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	10	0.92
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	3	0.92
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	3	0.92
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	3	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	3	0.92
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	3	0.92
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	3	0.92
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	6	0.92
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	5	0.92
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	5	0.92
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	10	0.92
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	10	0.92
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	3	0.92
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	3	0.92
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	3	0.92
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	3	0.92
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	3	0.92
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	3	0.92
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	6	0.92
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	2	0.92
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	5	0.92
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	5	0.92
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	5	0.92
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	5	0.92
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	5	0.92
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	5	0.92
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	7	0.92
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	7	0.92
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	7	0.92
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	10	0.92
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	10	0.92
(1,284)	1:18:A:SER:H	1:19:A:SER:H	10	0.92
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	8	0.92
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	8	0.92
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.92
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	8	0.92
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.92
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	9	0.92
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	9	0.92
(1,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	9	0.92
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	5	0.92
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	9	0.91
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	2	0.91
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	2	0.91
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	2	0.91
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	6	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	6	0.91
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	6	0.91
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	5	0.91
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	1	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	10	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	10	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	10	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	10	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	10	0.91
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	10	0.91
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	6	0.91
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	1	0.91
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	1	0.91
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	3	0.91
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	6	0.9
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	6	0.9
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	6	0.9
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	6	0.9
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	6	0.9
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	6	0.9
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.9
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	3	0.9
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	6	0.9
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.9
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	6	0.9
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	6	0.9
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	6	0.9
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	6	0.9
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	6	0.9
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	6	0.9
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	3	0.9
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	6	0.9
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	1	0.9
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	1	0.9
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	3	0.9
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	6	0.9
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	3	0.9
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	3	0.9
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	3	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	3	0.9
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	3	0.9
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	3	0.9
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	3	0.9
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	10	0.9
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	10	0.9
(1,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	10	0.9
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	5	0.9
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	5	0.9
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	5	0.9
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	5	0.9
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	5	0.9
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	5	0.9
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	10	0.9
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	10	0.9
(1,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	10	0.9
(1,284)	1:18:A:SER:H	1:19:A:SER:H	3	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	3	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	3	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	3	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	3	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	6	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	6	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	6	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	6	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	10	0.9
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	10	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	10	0.9
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	10	0.9
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	1	0.9
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	5	0.9
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	5	0.9
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	5	0.9
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	3	0.89
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	3	0.89
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	3	0.89
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	3	0.89
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.89
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	8	0.89
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	3	0.89
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	3	0.89
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	3	0.89
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.89
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	8	0.89
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	4	0.89
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	7	0.89
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	4	0.89
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	8	0.89
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	5	0.89
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	1	0.89
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	9	0.88
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	9	0.88
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.88
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.88
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	10	0.88
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	10	0.88
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	10	0.88
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	10	0.88
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	10	0.88
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	10	0.88
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	9	0.88
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	9	0.88
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.88
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.88
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	4	0.88
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	5	0.88
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	7	0.88
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	2	0.88
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	9	0.88
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	9	0.88
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	9	0.88
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	6	0.88
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	6	0.88
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	6	0.88
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	1	0.88
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	1	0.88
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	1	0.88
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	1	0.88
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	1	0.88
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	1	0.88
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	5	0.88
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	7	0.88
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	4	0.88
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	1	0.87
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	1	0.87
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	2	0.87
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	2	0.87
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	2	0.87
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	2	0.87
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	2	0.87
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	2	0.87
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.87
(4,17)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.87
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.87
(4,17)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.87
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	1	0.87
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	1	0.87
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	2	0.87
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	2	0.87
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	2	0.87
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	2	0.87
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	2	0.87
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	2	0.87
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.87
(2,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.87
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.87
(2,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.87
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	10	0.87
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	10	0.87
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	10	0.87
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	10	0.87
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	10	0.87
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	10	0.87
(1,535)	1:3:A:GLU:HG3	1:7:A:LEU:H	8	0.87
(1,518)	1:16:A:GLY:HA3	1:17:A:PRO:HD3	4	0.87
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	7	0.87
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	7	0.87
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	6	0.87
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	1	0.87
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	10	0.87
(1,291)	1:19:A:SER:HB2	1:19:A:SER:HG	4	0.87
(1,291)	1:19:A:SER:HB3	1:19:A:SER:HG	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:18:A:SER:H	1:19:A:SER:H	7	0.87
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	8	0.87
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	10	0.86
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	10	0.86
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	10	0.86
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	10	0.86
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	10	0.86
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	10	0.86
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	5	0.86
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.86
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	10	0.86
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	10	0.86
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	10	0.86
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	10	0.86
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	10	0.86
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	10	0.86
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	5	0.86
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.86
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	4	0.86
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	4	0.86
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	6	0.86
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	2	0.86
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	2	0.86
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	2	0.86
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	2	0.86
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	2	0.86
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	2	0.86
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	5	0.86
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	2	0.86
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	3	0.86
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	8	0.86
(1,284)	1:18:A:SER:H	1:19:A:SER:H	2	0.86
(1,284)	1:18:A:SER:H	1:19:A:SER:H	5	0.86
(1,254)	1:14:A:GLN:HA	1:14:A:GLN:HE21	10	0.86
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	9	0.86
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	2	0.86
(1,44)	1:6:A:ARG:HA	1:6:A:ARG:HG3	8	0.86
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	8	0.85
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	8	0.85
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	5	0.85
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	9	0.85
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	9	0.85
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	9	0.85
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	3	0.85
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	3	0.85
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	4	0.85
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	9	0.85
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	4	0.85
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	4	0.85
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	4	0.85
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	1	0.85
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	1	0.85
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	1	0.85
(1,436)	1:11:A:TRP:HB3	1:11:A:TRP:HE3	1	0.85
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	10	0.85
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	1	0.85
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	7	0.85
(1,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	8	0.85
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	4	0.84
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	4	0.84
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	4	0.84
(3,185)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.84
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	4	0.84
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	4	0.84
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	4	0.84
(2,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.84
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	2	0.84
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	2	0.84
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	4	0.84
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	4	0.84
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	6	0.84
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	7	0.84
(1,330)	1:23:A:PRO:HA	1:23:A:PRO:HB3	9	0.84
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	3	0.84
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	6	0.84
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	6	0.84
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG2	3	0.84
(1,250)	1:13:A:LYS:H	1:13:A:LYS:HG3	3	0.84
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	3	0.84
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	2	0.84
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	4	0.84
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	6	0.84
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	9	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	8	0.84
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	2	0.84
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	3	0.84
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	6	0.84
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	7	0.84
(1,51)	1:6:A:ARG:HB3	1:6:A:ARG:HE	9	0.84
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	2	0.84
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	1	0.83
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	2	0.83
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	4	0.83
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	4	0.83
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	4	0.83
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	4	0.83
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	4	0.83
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	4	0.83
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	5	0.83
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	8	0.83
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	1	0.83
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	5	0.83
(1,284)	1:18:A:SER:H	1:19:A:SER:H	6	0.83
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	9	0.83
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	9	0.83
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	9	0.83
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	9	0.83
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	4	0.83
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	3	0.83
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	5	0.83
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	8	0.83
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	10	0.83
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	8	0.83
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	2	0.82
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	2	0.82
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	1	0.82
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	1	0.82
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	1	0.82
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	2	0.82
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	2	0.82
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	2	0.82
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	2	0.82
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	2	0.82
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	3	0.82
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	3	0.82
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	8	0.82
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	8	0.82
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	8	0.82
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	8	0.82
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	1	0.82
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	8	0.82
(1,135)	1:22:A:PRO:HA	1:22:A:PRO:HB3	10	0.82
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	7	0.82
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	5	0.81
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	5	0.81
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	1	0.81
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	1	0.81
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	1	0.81
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	1	0.81
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	7	0.81
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	2	0.81
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	2	0.81
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	5	0.81
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	7	0.81
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	3	0.81
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	3	0.81
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	7	0.81
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	7	0.81
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	7	0.81
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	7	0.81
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	7	0.81
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	7	0.81
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	2	0.81
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	2	0.81
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	2	0.81
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	2	0.81
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	7	0.81
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	9	0.81
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	2	0.81
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	7	0.81
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	9	0.81
(1,299)	1:21:A:ARG:HA	1:21:A:ARG:HG3	9	0.81
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	3	0.81
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	3	0.81
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	3	0.81
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	6	0.8
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	6	0.8
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	6	0.8
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	6	0.8
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	6	0.8
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	6	0.8
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	6	0.8
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	6	0.8
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	6	0.8
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	6	0.8
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	6	0.8
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	4	0.8
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	5	0.8
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	5	0.8
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	1	0.8
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	1	0.8
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	1	0.8
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	1	0.8
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	1	0.8
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	2	0.8
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	6	0.8
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	9	0.8
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	4	0.8
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	2	0.8
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	2	0.8
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	2	0.8
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	2	0.8
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	7	0.8
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	7	0.8
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	7	0.8
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	7	0.79
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	7	0.79
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	7	0.79
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	7	0.79
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	7	0.79
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	7	0.79
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.79
(3,410)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.79
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.79
(2,454)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.79
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	7	0.79
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	7	0.79
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	7	0.79
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	7	0.79
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	7	0.79
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	7	0.79
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	9	0.79
(1,500)	1:12:A:LEU:HD21	1:16:A:GLY:HA2	10	0.79
(1,500)	1:12:A:LEU:HD22	1:16:A:GLY:HA2	10	0.79
(1,500)	1:12:A:LEU:HD23	1:16:A:GLY:HA2	10	0.79
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	9	0.79
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	9	0.79
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	9	0.79
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	9	0.79
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	9	0.79
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	9	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	1	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	5	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	7	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	8	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	9	0.79
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	10	0.79
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	1	0.79
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	7	0.79
(1,328)	1:23:A:PRO:HB3	1:23:A:PRO:HG3	6	0.79
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	3	0.79
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD2	4	0.79
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD3	4	0.79
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	9	0.79
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	9	0.79
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	9	0.79
(1,198)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	5	0.79
(1,194)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	10	0.79
(1,194)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	10	0.79
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	4	0.78
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	4	0.78
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	1	0.78
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	1	0.78
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	1	0.78
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.78
(3,83)	1:6:A:ARG:H	1:7:A:LEU:HD11	8	0.78
(3,83)	1:6:A:ARG:H	1:7:A:LEU:HD12	8	0.78
(3,83)	1:6:A:ARG:H	1:7:A:LEU:HD13	8	0.78
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	1	0.78
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	1	0.78
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	1	0.78
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.78
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	4	0.78
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	4	0.78
(2,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	8	0.78
(2,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	8	0.78
(2,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	8	0.78
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	7	0.78
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	7	0.78
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	2	0.78
(1,490)	1:6:A:ARG:HA	1:9:A:ILE:HB	3	0.78
(1,419)	1:16:A:GLY:HA2	1:16:A:GLY:HA3	3	0.78
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	5	0.78
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	3	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	3	0.78
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	3	0.78
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	5	0.78
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	5	0.78
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	5	0.78
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	1	0.78
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	9	0.78
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.77
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.77
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.77
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.77
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.77
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.77
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.77
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.77
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.77
(3,356)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.77
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.77
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.77
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.77
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.77
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.77
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.77
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.77
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.77
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.77
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.77
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.77
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.77
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.77
(2,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.77
(1,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	6	0.77
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	7	0.77
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	7	0.77
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	3	0.77
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	3	0.77
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	9	0.77
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	9	0.77
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	9	0.77
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	2	0.77
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	10	0.77
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	9	0.77
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	9	0.77
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	7	0.77
(1,284)	1:18:A:SER:H	1:19:A:SER:H	4	0.77
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	4	0.77
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	4	0.77
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	4	0.77
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	1	0.77
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	2	0.76
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	8	0.76
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	8	0.76
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	8	0.76
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	4	0.76
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	2	0.76
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	8	0.76
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	8	0.76
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	8	0.76
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	4	0.76
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	8	0.76
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	5	0.76
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	5	0.76
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	5	0.76
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	5	0.76
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	5	0.76
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	5	0.76
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	7	0.76
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	1	0.76
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	1	0.76
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	7	0.76
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	7	0.76
(1,185)	1:9:A:ILE:H	1:9:A:ILE:HG12	8	0.76
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	6	0.75
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	8	0.75
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	8	0.75
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	8	0.75
(3,50)	1:5:A:VAL:H	1:6:A:ARG:HG2	3	0.75
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	6	0.75
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	8	0.75
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	8	0.75
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	8	0.75
(2,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	3	0.75
(1,542)	1:17:A:PRO:HG2	1:18:A:SER:H	1	0.75
(1,542)	1:17:A:PRO:HG3	1:18:A:SER:H	1	0.75
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	8	0.75
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	4	0.75
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	4	0.75
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	4	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	2	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	2	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	3	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	3	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	5	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	5	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	6	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	6	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	8	0.75
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	8	0.75
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	4	0.75
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	6	0.75
(1,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	1	0.75
(1,198)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	9	0.75
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.75
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	5	0.75
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	7	0.75
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	8	0.74
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	8	0.74
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	8	0.74
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	8	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	8	0.74
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	8	0.74
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	8	0.74
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	3	0.74
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	3	0.74
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	3	0.74
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	3	0.74
(1,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	4	0.74
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	10	0.74
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	1	0.74
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	1	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	5	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	5	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	5	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	7	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	7	0.74
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	7	0.74
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	5	0.74
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	4	0.74
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	4	0.74
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG2	10	0.74
(1,318)	1:22:A:PRO:HD3	1:22:A:PRO:HG3	10	0.74
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	10	0.74
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	10	0.74
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	10	0.74
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	9	0.74
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	1	0.74
(1,72)	1:6:A:ARG:H	1:7:A:LEU:H	10	0.74
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	10	0.74
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	5	0.74
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	2	0.73
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	2	0.73
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	2	0.73
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	8	0.73
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	8	0.73
(3,420)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	8	0.73
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	2	0.73
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	2	0.73
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	2	0.73
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	8	0.73
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	8	0.73
(2,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	10	0.73
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	10	0.73
(1,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	4	0.73
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	3	0.73
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	6	0.73
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	8	0.73
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	7	0.73
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	7	0.73
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	7	0.73
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	7	0.73
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	5	0.73
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	7	0.73
(1,198)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	8	0.73
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	5	0.73
(4,61)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	0.72
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	7	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.72
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.72
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	7	0.72
(2,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	3	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	3	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	3	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	4	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	4	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	4	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	5	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	5	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	5	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	10	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	10	0.72
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	10	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:18:A:SER:HB2	1:21:A:ARG:H	6	0.72
(1,532)	1:18:A:SER:HB3	1:21:A:ARG:H	6	0.72
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	10	0.72
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	10	0.72
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	10	0.72
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	10	0.72
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	10	0.72
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	10	0.72
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	1	0.72
(1,315)	1:21:A:ARG:H	1:21:A:ARG:HG3	10	0.72
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	2	0.72
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	2	0.72
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	10	0.71
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	8	0.71
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	8	0.71
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	9	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	1	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	1	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	1	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	2	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	2	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	2	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.71
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.71
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	3	0.71
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	9	0.71
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	10	0.71
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	8	0.71
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	8	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	1	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	1	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	1	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	2	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	2	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	2	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	7	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	7	0.71
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	7	0.71
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	3	0.71
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	1	0.71
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	6	0.71
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	7	0.71
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	2	0.71
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	2	0.71
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	3	0.71
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	3	0.71
(1,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	6	0.71
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	10	0.71
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	10	0.71
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	10	0.71
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	8	0.71
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	7	0.71
(1,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	8	0.71
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	8	0.71
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	10	0.71
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	3	0.71
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	5	0.71
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	10	0.71
(1,22)	1:3:A:GLU:HB2	1:4:A:ALA:H	6	0.71
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	1	0.7
(3,477)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.7
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.7
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.7
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.7
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	1	0.7
(2,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	4	0.7
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	9	0.7
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	9	0.7
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	9	0.7
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	5	0.7
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	1	0.7
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	1	0.7
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	8	0.7
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	4	0.7
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	9	0.7
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	1	0.7
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	2	0.7
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	1	0.7
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	4	0.69
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	4	0.69
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	4	0.69
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	4	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	4	0.69
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	4	0.69
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	4	0.69
(3,186)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.69
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.69
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.69
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.69
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	4	0.69
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	4	0.69
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	4	0.69
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	4	0.69
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	4	0.69
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	4	0.69
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	4	0.69
(2,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.69
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	6	0.69
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	6	0.69
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	6	0.69
(1,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	8	0.69
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	7	0.69
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	4	0.69
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	4	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	6	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	6	0.69
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	6	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	6	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	6	0.69
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	6	0.69
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	4	0.69
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	3	0.69
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	8	0.69
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	3	0.69
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	3	0.69
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	6	0.69
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	7	0.69
(3,428)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.68
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.68
(2,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	4	0.68
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	8	0.68
(1,524)	1:11:A:TRP:HD1	1:21:A:ARG:HB3	5	0.68
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	3	0.68
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	10	0.68
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	10	0.68
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	10	0.68
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	10	0.68
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	10	0.68
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	10	0.68
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	5	0.68
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	5	0.68
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	1	0.68
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	3	0.68
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	5	0.68
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	10	0.68
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	9	0.68
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	3	0.68
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	8	0.68
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	8	0.68
(1,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	8	0.68
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	4	0.68
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	9	0.68
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	7	0.67
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	2	0.67
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	2	0.67
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	6	0.67
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	6	0.67
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	6	0.67
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.67
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	8	0.67
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	8	0.67
(3,77)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	8	0.67
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	7	0.67
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	2	0.67
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	2	0.67
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	6	0.67
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	6	0.67
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	6	0.67
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	7	0.67
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD11	8	0.67
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD12	8	0.67
(2,84)	1:7:A:LEU:HB2	1:7:A:LEU:HD13	8	0.67
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	4	0.67
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	4	0.67
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	4	0.67
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	8	0.67
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	8	0.67
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	8	0.67
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	8	0.67
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	9	0.67
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	5	0.67
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	5	0.67
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	5	0.67
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	1	0.67
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	2	0.67
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	3	0.67
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	10	0.67
(1,198)	1:10:A:GLN:HE21	1:10:A:GLN:HG2	3	0.67
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	9	0.67
(1,194)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	6	0.67
(1,194)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	6	0.67
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	7	0.67
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	6	0.67
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	7	0.67
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.66
(3,413)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	2	0.66
(3,413)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	2	0.66
(3,50)	1:5:A:VAL:H	1:6:A:ARG:HG2	4	0.66
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	6	0.66
(2,457)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	2	0.66
(2,457)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	2	0.66
(2,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	4	0.66
(1,521)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	8	0.66
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	7	0.66
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	9	0.66
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	8	0.66
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	10	0.66
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	2	0.66
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	2	0.66
(1,408)	1:5:A:VAL:HG11	1:9:A:ILE:H	1	0.66
(1,408)	1:5:A:VAL:HG12	1:9:A:ILE:H	1	0.66
(1,408)	1:5:A:VAL:HG13	1:9:A:ILE:H	1	0.66
(1,408)	1:5:A:VAL:HG21	1:9:A:ILE:H	1	0.66
(1,408)	1:5:A:VAL:HG22	1:9:A:ILE:H	1	0.66
(1,408)	1:5:A:VAL:HG23	1:9:A:ILE:H	1	0.66
(1,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	1	0.66
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG2	1	0.66
(1,245)	1:13:A:LYS:HE2	1:13:A:LYS:HG3	1	0.66
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG2	1	0.66
(1,245)	1:13:A:LYS:HE3	1:13:A:LYS:HG3	1	0.66
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	1	0.66
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	1	0.66
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.66
(4,54)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	8	0.65
(4,54)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	8	0.65
(4,54)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	8	0.65
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	7	0.65
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	7	0.65
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	7	0.65
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	7	0.65
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	7	0.65
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	7	0.65
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	7	0.65
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	7	0.65
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.65
(2,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	8	0.65
(2,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	8	0.65
(2,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	8	0.65
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	2	0.65
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	7	0.65
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	7	0.65
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	7	0.65
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	7	0.65
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	7	0.65
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	7	0.65
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	7	0.65
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	7	0.65
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	7	0.65
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	7	0.65
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	7	0.65
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	7	0.65
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	10	0.65
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	5	0.65
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	5	0.65
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	5	0.65
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	5	0.65
(1,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	6	0.65
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	5	0.65
(1,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	4	0.65
(1,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	4	0.65
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	6	0.65
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	6	0.65
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	6	0.65
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	6	0.65
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	6	0.65
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	6	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	1	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	1	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	2	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	2	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	3	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	3	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	5	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	5	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	6	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	6	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	7	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	7	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	8	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	8	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	9	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	9	0.65
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	10	0.65
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	1	0.65
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	7	0.65
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	5	0.65
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	4	0.65
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	10	0.65
(1,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	5	0.65
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	2	0.64
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	2	0.64
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	6	0.64
(4,50)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	6	0.64
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.64
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	2	0.64
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	2	0.64
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	6	0.64
(2,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	6	0.64
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	5	0.64
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	2	0.64
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	2	0.64
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	2	0.64
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	2	0.64
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	3	0.64
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	5	0.64
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	5	0.64
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	10	0.64
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	10	0.64
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	2	0.64
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	3	0.64
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	3	0.64
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	2	0.64
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	6	0.64
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	1	0.64
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	1	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	5	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	5	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	5	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	5	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	5	0.64
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	5	0.64
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG2	4	0.64
(1,317)	1:22:A:PRO:HD2	1:22:A:PRO:HG3	4	0.64
(1,224)	1:12:A:LEU:H	1:12:A:LEU:HG	2	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	6	0.64
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	7	0.64
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	3	0.64
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	6	0.64
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	4	0.64
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	10	0.64
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	10	0.63
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	10	0.63
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	10	0.63
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	9	0.63
(3,211)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.63
(3,211)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.63
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	9	0.63
(2,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	4	0.63
(2,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	6	0.63
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	10	0.63
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	10	0.63
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	10	0.63
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	6	0.63
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	6	0.63
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	6	0.63
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	9	0.63
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	5	0.63
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	3	0.63
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	3	0.63
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	3	0.63
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	2	0.63
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	1	0.63
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	5	0.63
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	10	0.63
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	5	0.63
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	5	0.63
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	3	0.63
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.62
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.62
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.62
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	2	0.62
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	2	0.62
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	7	0.62
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	7	0.62
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	7	0.62
(1,565)	1:12:A:LEU:H	1:13:A:LYS:H	1	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	6	0.62
(1,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	6	0.62
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	4	0.62
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	4	0.62
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	4	0.62
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	4	0.62
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	4	0.62
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	4	0.62
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	4	0.62
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	4	0.62
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	4	0.62
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	10	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	1	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	2	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	3	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	4	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	5	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	6	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	7	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	8	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	9	0.62
(1,327)	1:23:A:PRO:HB2	1:23:A:PRO:HB3	10	0.62
(1,285)	1:17:A:PRO:HA	1:18:A:SER:H	10	0.62
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	9	0.62
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	8	0.62
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	8	0.62
(1,59)	1:6:A:ARG:HB3	1:6:A:ARG:HD2	3	0.62
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.61
(3,211)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.61
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	1	0.61
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	9	0.61
(2,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	2	0.61
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	1	0.61
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	8	0.61
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	6	0.61
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	6	0.61
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	6	0.61
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	6	0.61
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	6	0.61
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	9	0.61
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG11	5	0.61
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG12	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG13	5	0.61
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG21	5	0.61
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG22	5	0.61
(1,404)	1:3:A:GLU:H	1:5:A:VAL:HG23	5	0.61
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	1	0.61
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	10	0.61
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	5	0.61
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	3	0.61
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	3	0.6
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	3	0.6
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	3	0.6
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.6
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.6
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.6
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.6
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	2	0.6
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	6	0.6
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	10	0.6
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	3	0.6
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	3	0.6
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	3	0.6
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	2	0.6
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	6	0.6
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	6	0.6
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	6	0.6
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	10	0.6
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	4	0.6
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	4	0.6
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	4	0.6
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	4	0.6
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	4	0.6
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	4	0.6
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	3	0.6
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	5	0.6
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	5	0.6
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	9	0.6
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	8	0.6
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	2	0.6
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	2	0.6
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	2	0.6
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	6	0.6
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	1	0.6
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	1	0.6
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	5	0.6
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	5	0.6
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	7	0.6
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	7	0.6
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	6	0.6
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	6	0.59
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.59
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.59
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.59
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	8	0.59
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.59
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	2	0.59
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	6	0.59
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	3	0.59
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	7	0.59
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	8	0.59
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	8	0.59
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	10	0.59
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	2	0.59
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	3	0.59
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	4	0.59
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	8	0.59
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	8	0.59
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	3	0.59
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	3	0.59
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	3	0.59
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	8	0.59
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	7	0.59
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	8	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	3	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	4	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	5	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	6	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	7	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	8	0.59
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	10	0.59
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	10	0.59
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	6	0.59
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	4	0.59
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	10	0.59
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	10	0.59
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	6	0.59
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	6	0.59
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.58
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.58
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	1	0.58
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	1	0.58
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	1	0.58
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	1	0.58
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	1	0.58
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	1	0.58
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.58
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.58
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	7	0.58
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	2	0.58
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	5	0.58
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	1	0.58
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	1	0.58
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	1	0.58
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	1	0.58
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	1	0.58
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	1	0.58
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	2	0.58
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	2	0.58
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	7	0.58
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	7	0.58
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	7	0.58
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	7	0.58
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	7	0.58
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	9	0.58
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	9	0.58
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	10	0.58
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	10	0.58
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	5	0.58
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	7	0.58
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	9	0.58
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	10	0.58
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	10	0.58
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	1	0.58
(1,276)	1:17:A:PRO:HA	1:17:A:PRO:HB3	9	0.58
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	2	0.58
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	2	0.58
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	8	0.58
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	8	0.58
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	9	0.58
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.57
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.57
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.57
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	4	0.57
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	4	0.57
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.57
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.57
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.57
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.57
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.57
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.57
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	4	0.57
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	4	0.57
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	6	0.57
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	6	0.57
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	4	0.57
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	4	0.57
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	4	0.57
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	4	0.57
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	10	0.57
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	7	0.57
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	10	0.57
(1,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	8	0.57
(1,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	8	0.57
(1,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	8	0.57
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	10	0.57
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	8	0.57
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	8	0.57
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	8	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	3	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	3	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	3	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	3	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	3	0.57
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	3	0.57
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	2	0.57
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	2	0.57
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	2	0.57
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	2	0.57
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	2	0.57
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	8	0.57
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	8	0.57
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	1	0.57
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	3	0.57
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	8	0.57
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	1	0.57
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	3	0.57
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	5	0.57
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	5	0.57
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	6	0.57
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	8	0.57
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	8	0.57
(1,57)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	8	0.57
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	7	0.57
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	6	0.57
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	4	0.56
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	5	0.56
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	7	0.56
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	1	0.56
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	1	0.56
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	1	0.56
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	1	0.56
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	1	0.56
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	1	0.56
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	1	0.56
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	1	0.56
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.56
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.56
(3,438)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.56
(3,438)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.56
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	3	0.56
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.56
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.56
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	1	0.56
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	4	0.56
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	5	0.56
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	7	0.56
(2,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	8	0.56
(2,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	8	0.56
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	1	0.56
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	1	0.56
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	1	0.56
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	1	0.56
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	1	0.56
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	1	0.56
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	1	0.56
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	1	0.56
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	3	0.56
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	5	0.56
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	9	0.56
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	10	0.56
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	10	0.56
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	10	0.56
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	1	0.56
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	9	0.56
(1,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	1	0.56
(1,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	2	0.56
(1,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	2	0.56
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	3	0.56
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	6	0.56
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	10	0.56
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	1	0.56
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	1	0.56
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	1	0.56
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	5	0.56
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	10	0.56
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	10	0.56
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	9	0.56
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	1	0.56
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	1	0.56
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	10	0.56
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	10	0.56
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.55
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.55
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	9	0.55
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	7	0.55
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB2	10	0.55
(1,546)	1:18:A:SER:HB2	1:19:A:SER:HB3	10	0.55
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB2	10	0.55
(1,546)	1:18:A:SER:HB3	1:19:A:SER:HB3	10	0.55
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	2	0.55
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	2	0.55
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	2	0.55
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	2	0.55
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	2	0.55
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	2	0.55
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	3	0.55
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	3	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG11	4	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG12	4	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG13	4	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG21	4	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG22	4	0.55
(1,421)	1:3:A:GLU:HG2	1:5:A:VAL:HG23	4	0.55
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	4	0.55
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.55
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	3	0.55
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	3	0.55
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	3	0.55
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	10	0.55
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	10	0.55
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	10	0.55
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	10	0.55
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	5	0.55
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	4	0.55
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	3	0.55
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	3	0.55
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	2	0.55
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	2	0.55
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	4	0.55
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	4	0.55
(1,124)	1:21:A:ARG:HD2	1:21:A:ARG:HE	9	0.55
(1,124)	1:21:A:ARG:HD3	1:21:A:ARG:HE	9	0.55
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	4	0.55
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.54
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	4	0.54
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.54
(3,18)	1:3:A:GLU:HB3	1:4:A:ALA:H	8	0.54
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	4	0.54
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	8	0.54
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	7	0.54
(2,21)	1:3:A:GLU:HB3	1:4:A:ALA:H	8	0.54
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	7	0.54
(1,523)	1:11:A:TRP:HZ3	1:12:A:LEU:HG	8	0.54
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	4	0.54
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	4	0.54
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	4	0.54
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	4	0.54
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	4	0.54
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	4	0.54
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	10	0.54
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	10	0.54
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	10	0.54
(1,408)	1:5:A:VAL:HG11	1:9:A:ILE:H	2	0.54
(1,408)	1:5:A:VAL:HG12	1:9:A:ILE:H	2	0.54
(1,408)	1:5:A:VAL:HG13	1:9:A:ILE:H	2	0.54
(1,408)	1:5:A:VAL:HG21	1:9:A:ILE:H	2	0.54
(1,408)	1:5:A:VAL:HG22	1:9:A:ILE:H	2	0.54
(1,408)	1:5:A:VAL:HG23	1:9:A:ILE:H	2	0.54
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	2	0.54
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	7	0.54
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	2	0.54
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	3	0.54
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	1	0.54
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.53
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.53
(3,94)	1:7:A:LEU:HB2	1:8:A:TYR:H	6	0.53
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	10	0.53
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	3	0.53
(2,105)	1:7:A:LEU:HB2	1:8:A:TYR:H	6	0.53
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	1	0.53
(1,483)	1:13:A:LYS:H	1:14:A:GLN:HG2	4	0.53
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	7	0.53
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	7	0.53
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	7	0.53
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	7	0.53
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	7	0.53
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	7	0.53
(1,403)	1:3:A:GLU:H	1:5:A:VAL:HB	5	0.53
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	4	0.53
(1,342)	1:24:A:PRO:HD3	1:24:A:PRO:HG3	6	0.53
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	4	0.53
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	4	0.53
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	3	0.52
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	3	0.52
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.52
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.52
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.52
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	3	0.52
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	3	0.52
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	8	0.52
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	3	0.52
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	8	0.52
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	8	0.52
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	3	0.52
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	2	0.52
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	2	0.52
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	2	0.52
(1,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB3	1	0.52
(1,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB3	1	0.52
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	2	0.52
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	9	0.52
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	9	0.52
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	9	0.52
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	1	0.52
(1,224)	1:12:A:LEU:H	1:12:A:LEU:HG	4	0.52
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	8	0.52
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	9	0.52
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	9	0.52
(1,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	2	0.52
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	9	0.52
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	9	0.52
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	4	0.52
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	9	0.52
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	3	0.52
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	2	0.51
(4,55)	1:17:A:PRO:HA	1:17:A:PRO:HD3	6	0.51
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	2	0.51
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	2	0.51
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	1	0.51
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	1	0.51
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	1	0.51
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.51
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.51
(3,434)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.51
(3,434)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.51
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	3	0.51
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	3	0.51
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.51
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	3	0.51
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	9	0.51
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	2	0.51
(2,515)	1:17:A:PRO:HA	1:17:A:PRO:HD3	6	0.51
(2,479)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	2	0.51
(2,479)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	2	0.51
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	2	0.51
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	2	0.51
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	3	0.51
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	3	0.51
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	1	0.51
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	1	0.51
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	1	0.51
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	7	0.51
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	4	0.51
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	4	0.51
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	4	0.51
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	7	0.51
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	7	0.51
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	4	0.51
(1,339)	1:24:A:PRO:HD2	1:24:A:PRO:HG2	6	0.51
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	2	0.51
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	7	0.51
(1,224)	1:12:A:LEU:H	1:12:A:LEU:HG	6	0.51
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	7	0.51
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	3	0.51
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	3	0.51
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	3	0.51
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	7	0.51
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	7	0.51
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	4	0.51
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	4	0.5
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	9	0.5
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	10	0.5
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.5
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	4	0.5
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	9	0.5
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	10	0.5
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	7	0.5
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	4	0.5
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	4	0.5
(1,508)	1:11:A:TRP:H	1:12:A:LEU:HB3	3	0.5
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	5	0.5
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	7	0.5
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	7	0.5
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	9	0.5
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	9	0.5
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	6	0.5
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	8	0.5
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.5
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	6	0.5
(1,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.5
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	5	0.5
(4,66)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.49
(4,29)	1:24:A:PRO:HA	1:25:A:SER:H	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	1	0.49
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	2	0.49
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	3	0.49
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	7	0.49
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.49
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	1	0.49
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.49
(2,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	6	0.49
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	7	0.49
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	1	0.49
(2,363)	1:24:A:PRO:HA	1:25:A:SER:H	7	0.49
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	2	0.49
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	1	0.49
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	2	0.49
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	3	0.49
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	7	0.49
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	1	0.49
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	1	0.49
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	4	0.49
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	4	0.49
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	8	0.49
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	8	0.49
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	8	0.49
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	8	0.49
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	8	0.49
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	8	0.49
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	6	0.49
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	6	0.49
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	2	0.49
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	2	0.49
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	2	0.49
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	2	0.49
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	1	0.49
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	1	0.49
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	1	0.49
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	1	0.49
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	8	0.49
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	8	0.49
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	8	0.49
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	8	0.49
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	5	0.49
(1,190)	1:19:A:SER:H	1:19:A:SER:HG	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:25:A:SER:H	1:25:A:SER:HA	3	0.49
(1,121)	1:25:A:SER:H	1:25:A:SER:HA	9	0.49
(1,64)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	9	0.49
(1,58)	1:6:A:ARG:HB2	1:6:A:ARG:HD2	6	0.49
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	7	0.48
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	9	0.48
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	2	0.48
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	2	0.48
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	2	0.48
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	2	0.48
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	2	0.48
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	2	0.48
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	2	0.48
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	2	0.48
(4,10)	1:6:A:ARG:H	1:7:A:LEU:HB3	8	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.48
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.48
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	5	0.48
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	9	0.48
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	10	0.48
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	5	0.48
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.48
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	7	0.48
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.48
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	7	0.48
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	7	0.48
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.48
(3,43)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	5	0.48
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	5	0.48
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	7	0.48
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	7	0.48
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	9	0.48
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	2	0.48
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	2	0.48
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	2	0.48
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	2	0.48
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	2	0.48
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	2	0.48
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	2	0.48
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	2	0.48
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	4	0.48
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	7	0.48
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	7	0.48
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	4	0.48
(2,91)	1:6:A:ARG:H	1:7:A:LEU:HB3	8	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	1	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	1	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	1	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	4	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	4	0.48
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	4	0.48
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	5	0.48
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	9	0.48
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	10	0.48
(2,47)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.48
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	10	0.48
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	10	0.48
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	1	0.48
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	1	0.48
(1,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	2	0.48
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	3	0.48
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	7	0.48
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	7	0.48
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	7	0.48
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	7	0.48
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	7	0.48
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	7	0.48
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	8	0.48
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	8	0.48
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	2	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	4	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	4	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	4	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	4	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	6	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	6	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	6	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	6	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	10	0.48
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	10	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	10	0.48
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	10	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	5	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	5	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	5	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	5	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	7	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	7	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	7	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	7	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	9	0.48
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	9	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	9	0.48
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	9	0.48
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	10	0.48
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.48
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	0.48
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	7	0.48
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	8	0.48
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	8	0.48
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	8	0.48
(1,121)	1:25:A:SER:H	1:25:A:SER:HA	7	0.48
(1,40)	1:5:A:VAL:H	1:6:A:ARG:H	2	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	3	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	3	0.48
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	3	0.48
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	8	0.48
(4,29)	1:24:A:PRO:HA	1:25:A:SER:H	9	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.47
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.47
(4,5)	1:7:A:LEU:HA	1:7:A:LEU:HG	6	0.47
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.47
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	5	0.47
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.47
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	8	0.47
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.47
(2,363)	1:24:A:PRO:HA	1:25:A:SER:H	9	0.47
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	2	0.47
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	5	0.47
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	7	0.47
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	8	0.47
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	9	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	2	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	2	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	2	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	3	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	3	0.47
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	3	0.47
(2,75)	1:7:A:LEU:HA	1:7:A:LEU:HG	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	1	0.47
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	3	0.47
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	4	0.47
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	6	0.47
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	9	0.47
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	9	0.47
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	6	0.47
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	6	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	1	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	1	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	1	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	1	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	1	0.47
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	1	0.47
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	1	0.47
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	1	0.47
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	1	0.47
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	4	0.47
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	2	0.47
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	2	0.47
(1,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	4	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	2	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	2	0.47
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	2	0.47
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	2	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	4	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	4	0.47
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	4	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE2	6	0.47
(1,244)	1:13:A:LYS:HD2	1:13:A:LYS:HE3	6	0.47
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE2	6	0.47
(1,244)	1:13:A:LYS:HD3	1:13:A:LYS:HE3	6	0.47
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	2	0.47
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	2	0.47
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	2	0.47
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	2	0.47
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	1	0.47
(1,169)	1:8:A:TYR:HB3	1:9:A:ILE:H	3	0.47
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	1	0.47
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	1	0.47
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	1	0.47
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	1	0.47
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	7	0.47
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	7	0.47
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	3	0.47
(1,64)	1:6:A:ARG:HD3	1:6:A:ARG:HG3	6	0.47
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	1	0.47
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	7	0.47
(1,57)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	5	0.47
(1,44)	1:6:A:ARG:HA	1:6:A:ARG:HG3	6	0.47
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	10	0.47
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	9	0.47
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	8	0.47
(4,65)	1:3:A:GLU:HB2	1:4:A:ALA:HA	9	0.46
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.46
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.46
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	9	0.46
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	9	0.46
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	9	0.46
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	9	0.46
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	9	0.46
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	9	0.46
(4,29)	1:24:A:PRO:HA	1:25:A:SER:H	3	0.46
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.46
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.46
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.46
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.46
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.46
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.46
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.46
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.46
(3,283)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.46
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	9	0.46
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	9	0.46
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.46
(2,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	9	0.46
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	1	0.46
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	1	0.46
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	9	0.46
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	9	0.46
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	9	0.46
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	9	0.46
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	9	0.46
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	9	0.46
(2,363)	1:24:A:PRO:HA	1:25:A:SER:H	3	0.46
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	1	0.46
(2,308)	1:21:A:ARG:HB3	1:21:A:ARG:HG2	6	0.46
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	9	0.46
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	9	0.46
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	5	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	1	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	1	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	1	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	3	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	3	0.46
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	3	0.46
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	9	0.46
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	10	0.46
(1,510)	1:11:A:TRP:H	1:11:A:TRP:HD1	8	0.46
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	7	0.46
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	7	0.46
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	7	0.46
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	7	0.46
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	7	0.46
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	7	0.46
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	1	0.46
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	8	0.46
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	6	0.46
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	6	0.46
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	6	0.46
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	6	0.46
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	6	0.46
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	3	0.46
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	3	0.46
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	3	0.46
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	3	0.46
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	3	0.46
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	3	0.46
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	3	0.46
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	10	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	1	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	2	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	3	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	4	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	5	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	6	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	7	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	8	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	9	0.46
(1,324)	1:22:A:PRO:HB2	1:22:A:PRO:HB3	10	0.46
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	2	0.46
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	2	0.46
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	2	0.46
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	3	0.46
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	3	0.46
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	2	0.46
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	2	0.46
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	10	0.46
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	10	0.46
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	6	0.46
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	6	0.46
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	6	0.46
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	4	0.46
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	2	0.46
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	2	0.46
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	7	0.46
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.45
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	5	0.45
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.45
(3,51)	1:6:A:ARG:HA	1:6:A:ARG:HD2	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	5	0.45
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	8	0.45
(2,55)	1:6:A:ARG:HA	1:6:A:ARG:HD2	5	0.45
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.45
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	7	0.45
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	2	0.45
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	8	0.45
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	3	0.45
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD21	10	0.45
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD22	10	0.45
(1,446)	1:11:A:TRP:HZ3	1:12:A:LEU:HD23	10	0.45
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	1	0.45
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	5	0.45
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	5	0.45
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	6	0.45
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	6	0.45
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	7	0.45
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	7	0.45
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	8	0.45
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	8	0.45
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	8	0.45
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	8	0.45
(1,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	8	0.45
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	7	0.45
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	6	0.45
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	6	0.45
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	10	0.45
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	1	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG11	4	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG12	4	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG13	4	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	4	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	4	0.45
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	4	0.45
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	5	0.44
(4,43)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	5	0.44
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	5	0.44
(4,43)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	5	0.44
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	5	0.44
(4,43)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	5	0.44
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.44
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.44
(3,461)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.44
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	6	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	8	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	8	0.44
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	8	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	8	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	8	0.44
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	8	0.44
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	5	0.44
(3,221)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	5	0.44
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.44
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.44
(2,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	10	0.44
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	6	0.44
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	8	0.44
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	8	0.44
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	8	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	8	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	8	0.44
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	8	0.44
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	5	0.44
(2,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	5	0.44
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	5	0.44
(2,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	5	0.44
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	5	0.44
(2,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	5	0.44
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	5	0.44
(2,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	5	0.44
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	8	0.44
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	10	0.44
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	5	0.44
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	5	0.44
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	5	0.44
(1,525)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.44
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	5	0.44
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	7	0.44
(1,456)	1:11:A:TRP:HD1	1:21:A:ARG:HB2	10	0.44
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	1	0.44
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	1	0.44
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	1	0.44
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	1	0.44
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	1	0.44
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	1	0.44
(1,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	10	0.44
(1,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	10	0.44
(1,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	10	0.44
(1,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	10	0.44
(1,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	10	0.44
(1,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	10	0.44
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG2	4	0.44
(1,394)	1:11:A:TRP:HH2	1:17:A:PRO:HG3	4	0.44
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	1	0.44
(1,382)	1:11:A:TRP:HE1	1:21:A:ARG:HB3	8	0.44
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	4	0.44
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	4	0.44
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	5	0.44
(1,331)	1:23:A:PRO:HA	1:23:A:PRO:HB2	8	0.44
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	9	0.44
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	1	0.44
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	1	0.44
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	8	0.44
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	8	0.44
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	4	0.44
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	4	0.44
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	8	0.44
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	8	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	3	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	3	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	3	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	3	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	5	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	5	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	5	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	5	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	7	0.44
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	7	0.44
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	7	0.44
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	1	0.44
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	1	0.44
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	1	0.44
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	4	0.44
(1,226)	1:12:A:LEU:HA	1:12:A:LEU:HB3	6	0.44
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	10	0.44
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	8	0.44
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	1	0.44
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	2	0.44
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	2	0.44
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	3	0.44
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	3	0.44
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	9	0.44
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	9	0.44
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	3	0.44
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	5	0.44
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	6	0.44
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	8	0.44
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	9	0.44
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	2	0.44
(1,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.44
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	4	0.43
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	4	0.43
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	4	0.43
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	4	0.43
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	4	0.43
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	4	0.43
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	4	0.43
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	4	0.43
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	1	0.43
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	1	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.43
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.43
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.43
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.43
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.43
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.43
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.43
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	9	0.43
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	4	0.43
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	4	0.43
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	4	0.43
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	4	0.43
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	4	0.43
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	4	0.43
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	4	0.43
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	4	0.43
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	1	0.43
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	1	0.43
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	1	0.43
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	2	0.43
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	2	0.43
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	2	0.43
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	10	0.43
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	5	0.43
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	5	0.43
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	5	0.43
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.43
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	9	0.43
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	6	0.43
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	7	0.43
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	7	0.43
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	3	0.43
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	3	0.43
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	3	0.43
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	3	0.43
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	3	0.43
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	3	0.43
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD21	8	0.43
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD22	8	0.43
(1,443)	1:6:A:ARG:HH11	1:7:A:LEU:HD23	8	0.43
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	7	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	2	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	2	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	2	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	2	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	2	0.43
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	2	0.43
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	2	0.43
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	2	0.43
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	8	0.43
(1,360)	1:6:A:ARG:HA	1:9:A:ILE:H	4	0.43
(1,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD3	9	0.43
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	9	0.43
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	9	0.43
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	9	0.43
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	9	0.43
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	5	0.43
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	5	0.43
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	2	0.43
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	2	0.43
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	7	0.43
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	10	0.43
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	7	0.43
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	10	0.43
(1,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.43
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	5	0.43
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	8	0.42
(4,51)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	10	0.42
(4,51)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	10	0.42
(4,36)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	9	0.42
(4,36)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	9	0.42
(4,36)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	9	0.42
(4,36)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	9	0.42
(4,36)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	9	0.42
(4,36)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	9	0.42
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	5	0.42
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	5	0.42
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	5	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.42
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.42
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.42
(4,7)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.42
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.42
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	7	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	9	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	9	0.42
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	9	0.42
(3,231)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.42
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.42
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	3	0.42
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	4	0.42
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	8	0.42
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	3	0.42
(2,504)	1:13:A:LYS:HG2	1:14:A:GLN:HB2	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,504)	1:13:A:LYS:HG3	1:14:A:GLN:HB2	10	0.42
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	7	0.42
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	9	0.42
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	9	0.42
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	9	0.42
(2,425)	1:5:A:VAL:HG11	1:6:A:ARG:HB2	9	0.42
(2,425)	1:5:A:VAL:HG12	1:6:A:ARG:HB2	9	0.42
(2,425)	1:5:A:VAL:HG13	1:6:A:ARG:HB2	9	0.42
(2,425)	1:5:A:VAL:HG21	1:6:A:ARG:HB2	9	0.42
(2,425)	1:5:A:VAL:HG22	1:6:A:ARG:HB2	9	0.42
(2,425)	1:5:A:VAL:HG23	1:6:A:ARG:HB2	9	0.42
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	5	0.42
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	5	0.42
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	5	0.42
(2,256)	1:14:A:GLN:H	1:14:A:GLN:HB2	3	0.42
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	2	0.42
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	3	0.42
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	4	0.42
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	6	0.42
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	8	0.42
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	3	0.42
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	6	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	6	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	6	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	6	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD21	9	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD22	9	0.42
(2,78)	1:7:A:LEU:HA	1:7:A:LEU:HD23	9	0.42
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	3	0.42
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	4	0.42
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	4	0.42
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	4	0.42
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	4	0.42
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	1	0.42
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	1	0.42
(1,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	1	0.42
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	10	0.42
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	4	0.42
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	4	0.42
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	4	0.42
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD2	4	0.42
(1,143)	1:23:A:PRO:HA	1:23:A:PRO:HD3	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	8	0.42
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	7	0.42
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	9	0.42
(1,63)	1:6:A:ARG:HD2	1:6:A:ARG:HG3	1	0.42
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	7	0.42
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.41
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	0.41
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	8	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	2	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	2	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	2	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	6	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	6	0.41
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	6	0.41
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.41
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.41
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.41
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	0.41
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.41
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.41
(4,15)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.41
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.41
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.41
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.41
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	5	0.41
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.41
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.41
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.41
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	2	0.41
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	2	0.41
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	8	0.41
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	5	0.41
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	9	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	2	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	2	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	2	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	6	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	6	0.41
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	6	0.41
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	2	0.41
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	6	0.41
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	6	0.41
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	6	0.41
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	1	0.41
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	5	0.41
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	7	0.41
(2,137)	1:22:A:PRO:HA	1:22:A:PRO:HD2	9	0.41
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	3	0.41
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	3	0.41
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	3	0.41
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	4	0.41
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	4	0.41
(1,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	4	0.41
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	4	0.41
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	4	0.41
(1,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	4	0.41
(1,437)	1:11:A:TRP:HE3	1:12:A:LEU:HB3	9	0.41
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	2	0.41
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	7	0.41
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	2	0.41
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	8	0.41
(1,311)	1:21:A:ARG:HB3	1:21:A:ARG:HE	8	0.41
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	10	0.41
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	10	0.41
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	5	0.41
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	5	0.41
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	10	0.41
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	6	0.41
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	7	0.4
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	7	0.4
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	7	0.4
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	7	0.4
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	7	0.4
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.4
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.4
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.4
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.4
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	2	0.4
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	2	0.4
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.4
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.4
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	2	0.4
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	7	0.4
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	7	0.4
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	2	0.4
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	7	0.4
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	7	0.4
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	6	0.4
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	5	0.4
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	10	0.4
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	10	0.4
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	10	0.4
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	7	0.4
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	6	0.4
(1,491)	1:21:A:ARG:HB2	1:22:A:PRO:HD3	9	0.4
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	10	0.4
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	10	0.4
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	3	0.4
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	5	0.4
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	5	0.4
(1,459)	1:23:A:PRO:HB2	1:25:A:SER:H	2	0.4
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	8	0.4
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	8	0.4
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	8	0.4
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	8	0.4
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	8	0.4
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	8	0.4
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	9	0.4
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	9	0.4
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	2	0.4
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	8	0.4
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	2	0.4
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	6	0.4
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD2	2	0.4
(1,242)	1:13:A:LYS:HA	1:13:A:LYS:HD3	2	0.4
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	3	0.4
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	4	0.4
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	6	0.4
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	2	0.4
(1,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	9	0.4
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	6	0.4
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	6	0.4
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	6	0.4
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	10	0.4
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	6	0.4
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	6	0.4
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	4	0.4
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	4	0.4
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	4	0.4
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	10	0.4
(1,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	8	0.4
(1,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	8	0.4
(1,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	8	0.4
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB1	9	0.4
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB2	9	0.4
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB3	9	0.4
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	5	0.39
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	5	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	3	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	3	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	3	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	4	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	4	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	4	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	9	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	9	0.39
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	9	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.39
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.39
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.39
(3,434)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.39
(3,434)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.39
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.39
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.39
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	9	0.39
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.39
(2,479)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	4	0.39
(2,479)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	4	0.39
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	5	0.39
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	5	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	3	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	3	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	4	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	4	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	4	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	9	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	9	0.39
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	9	0.39
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	4	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	4	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	4	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	4	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	5	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	5	0.39
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	5	0.39
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.39
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.39
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	9	0.39
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	1	0.39
(1,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	1	0.39
(1,447)	1:8:A:TYR:HD1	1:23:A:PRO:HB3	8	0.39
(1,447)	1:8:A:TYR:HD2	1:23:A:PRO:HB3	8	0.39
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	1	0.39
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	1	0.39
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	1	0.39
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	1	0.39
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	1	0.39
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	1	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	8	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	8	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	8	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	8	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	8	0.39
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	8	0.39
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	7	0.39
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	3	0.39
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	5	0.39
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD2	3	0.39
(1,301)	1:21:A:ARG:HB3	1:21:A:ARG:HD3	3	0.39
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	3	0.39
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	3	0.39
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	10	0.39
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	4	0.39
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	4	0.39
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	8	0.39
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	8	0.39
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	8	0.39
(1,213)	1:12:A:LEU:HA	1:16:A:GLY:H	9	0.39
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	4	0.39
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	1	0.39
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD2	4	0.39
(1,161)	1:11:A:TRP:HZ2	1:23:A:PRO:HD3	4	0.39
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	4	0.39
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	4	0.39
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	1	0.39
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	4	0.39
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	9	0.39
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.38
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.38
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	9	0.38
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	9	0.38
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	3	0.38
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	3	0.38
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	3	0.38
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	3	0.38
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	3	0.38
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	3	0.38
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	3	0.38
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	3	0.38
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.38
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.38
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.38
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,456)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.38
(3,456)	1:10:A:GLN:HB3	1:11:A:TRP:H	2	0.38
(3,455)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.38
(3,40)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.38
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	10	0.38
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	10	0.38
(2,507)	1:10:A:GLN:HB2	1:11:A:TRP:H	2	0.38
(2,507)	1:10:A:GLN:HB3	1:11:A:TRP:H	2	0.38
(2,506)	1:21:A:ARG:HB2	1:22:A:PRO:HD2	4	0.38
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	9	0.38
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	9	0.38
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	3	0.38
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	3	0.38
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	3	0.38
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	3	0.38
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	3	0.38
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	3	0.38
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	3	0.38
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	3	0.38
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	1	0.38
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	1	0.38
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.38
(2,43)	1:6:A:ARG:HA	1:6:A:ARG:HG2	5	0.38
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	8	0.38
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD11	1	0.38
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD12	1	0.38
(1,555)	1:9:A:ILE:HA	1:12:A:LEU:HD13	1	0.38
(1,553)	1:10:A:GLN:HA	1:13:A:LYS:HB2	1	0.38
(1,476)	1:13:A:LYS:HB2	1:14:A:GLN:H	8	0.38
(1,470)	1:3:A:GLU:H	1:5:A:VAL:H	6	0.38
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	9	0.38
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	9	0.38
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	9	0.38
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	9	0.38
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	9	0.38
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	9	0.38
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	9	0.38
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	9	0.38
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	9	0.38
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	9	0.38
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	9	0.38
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	9	0.38
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	9	0.38
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	1	0.38
(1,351)	1:23:A:PRO:HA	1:24:A:PRO:HD3	3	0.38
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	3	0.38
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	1	0.38
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	1	0.38
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	2	0.38
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	10	0.38
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG2	1	0.38
(1,247)	1:13:A:LYS:HB2	1:13:A:LYS:HG3	1	0.38
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG2	1	0.38
(1,247)	1:13:A:LYS:HB3	1:13:A:LYS:HG3	1	0.38
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	2	0.38
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	2	0.38
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	2	0.38
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	1	0.38
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	2	0.38
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	10	0.38
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	3	0.38
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	5	0.38
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.38
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	1	0.38
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	3	0.38
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	6	0.38
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	9	0.38
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	2	0.38
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	3	0.38
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	4	0.38
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	3	0.38
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.38
(1,1)	1:3:A:GLU:H	1:3:A:GLU:HA	6	0.38
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	1	0.37
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	1	0.37
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	1	0.37
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	2	0.37
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	2	0.37
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	2	0.37
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.37
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.37
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	0.37
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	0.37
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	0.37
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.37
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.37
(3,434)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.37
(3,434)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.37
(3,235)	1:14:A:GLN:H	1:14:A:GLN:HG3	10	0.37
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.37
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.37
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.37
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	5	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	1	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	1	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	1	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	2	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	2	0.37
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	2	0.37
(2,479)	1:8:A:TYR:HE1	1:12:A:LEU:HB3	6	0.37
(2,479)	1:8:A:TYR:HE2	1:12:A:LEU:HB3	6	0.37
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	7	0.37
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	9	0.37
(2,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	10	0.37
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	8	0.37
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	8	0.37
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	4	0.37
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	2	0.37
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	7	0.37
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	7	0.37
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	7	0.37
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.37
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.37
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	5	0.37
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	9	0.37
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	9	0.37
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	9	0.37
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	9	0.37
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	9	0.37
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	9	0.37
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	7	0.37
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	7	0.37
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	7	0.37
(1,550)	1:8:A:TYR:HA	1:24:A:PRO:HG2	8	0.37
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	7	0.37
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	9	0.37
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	9	0.37
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	9	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	2	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	3	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	5	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	6	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	7	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	8	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	9	0.37
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	10	0.37
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	3	0.37
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	3	0.37
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	3	0.37
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	3	0.37
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	8	0.37
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	8	0.37
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	8	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	3	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	4	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	5	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	6	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	8	0.37
(1,204)	1:11:A:TRP:HB2	1:11:A:TRP:HB3	9	0.37
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	7	0.37
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	9	0.37
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD2	8	0.37
(1,149)	1:23:A:PRO:HB3	1:23:A:PRO:HD3	8	0.37
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	3	0.37
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	3	0.37
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	3	0.37
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	2	0.37
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	3	0.37
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	4	0.37
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	10	0.37
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	9	0.37
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	10	0.37
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	4	0.37
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	10	0.36
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	0.36
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	0.36
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	0.36
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	6	0.36
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	6	0.36
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	6	0.36
(4,38)	1:13:A:LYS:HG2	1:14:A:GLN:HA	10	0.36
(4,38)	1:13:A:LYS:HG3	1:14:A:GLN:HA	10	0.36
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.36
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.36
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.36
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.36
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.36
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.36
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.36
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.36
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	3	0.36
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	3	0.36
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	3	0.36
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	3	0.36
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	3	0.36
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	8	0.36
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.36
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.36
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	10	0.36
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	8	0.36
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	8	0.36
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	8	0.36
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	6	0.36
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	6	0.36
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	6	0.36
(2,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	10	0.36
(2,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	10	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	3	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	3	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	3	0.36
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	3	0.36
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	3	0.36
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	3	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	3	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	3	0.36
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	3	0.36
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	3	0.36
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	3	0.36
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	3	0.36
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	3	0.36
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	5	0.36
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	6	0.36
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	8	0.36
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	8	0.36
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	3	0.36
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	4	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	7	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	7	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	7	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	10	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	10	0.36
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	10	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	1	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	1	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	1	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	2	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	2	0.36
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	2	0.36
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	10	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	4	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	4	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	4	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	4	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	4	0.36
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	4	0.36
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	1	0.36
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	1	0.36
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	10	0.36
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	4	0.36
(1,329)	1:23:A:PRO:HB3	1:23:A:PRO:HG2	6	0.36
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	9	0.36
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	2	0.36
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	2	0.36
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	6	0.36
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	1	0.36
(1,270)	1:15:A:GLY:HA2	1:15:A:GLY:HA3	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	3	0.36
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	3	0.36
(1,238)	1:13:A:LYS:H	1:13:A:LYS:HB2	1	0.36
(1,224)	1:12:A:LEU:H	1:12:A:LEU:HG	8	0.36
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	9	0.36
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	2	0.36
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	6	0.36
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	9	0.36
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	1	0.36
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	5	0.36
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	10	0.36
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	9	0.36
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	9	0.36
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	9	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	1	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	1	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	1	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	7	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	7	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	7	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	10	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	10	0.36
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	10	0.36
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	6	0.36
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	5	0.36
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	8	0.36
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	3	0.36
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	4	0.36
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	10	0.36
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	3	0.36
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	10	0.35
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	10	0.35
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	10	0.35
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	4	0.35
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	4	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	7	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	7	0.35
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	7	0.35
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	10	0.35
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	10	0.35
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	10	0.35
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	8	0.35
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	8	0.35
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.35
(4,6)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	4	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	4	0.35
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	4	0.35
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	4	0.35
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	4	0.35
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	6	0.35
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	7	0.35
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	10	0.35
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	10	0.35
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	10	0.35
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	4	0.35
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	4	0.35
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	7	0.35
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	7	0.35
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	7	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	4	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	4	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	4	0.35
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	4	0.35
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	4	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	4	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	4	0.35
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	4	0.35
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	4	0.35
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	4	0.35
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	4	0.35
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	4	0.35
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	10	0.35
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	10	0.35
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	10	0.35
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	8	0.35
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	8	0.35
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	8	0.35
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	6	0.35
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	3	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	6	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	6	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	6	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD11	9	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD12	9	0.35
(2,77)	1:7:A:LEU:HA	1:7:A:LEU:HD13	9	0.35
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	7	0.35
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	3	0.35
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	3	0.35
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	10	0.35
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	10	0.35
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	8	0.35
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	8	0.35
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	8	0.35
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	1	0.35
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	5	0.35
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	10	0.35
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	4	0.35
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	4	0.35
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	5	0.35
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	4	0.35
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	5	0.35
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	6	0.35
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	7	0.35
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	8	0.35
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.35
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	9	0.35
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	10	0.35
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	6	0.35
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	4	0.35
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	4	0.35
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	0.35
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	4	0.35
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	4	0.35
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	4	0.35
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	4	0.35
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	8	0.35
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	3	0.35
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	5	0.35
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	7	0.35
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	7	0.35
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	7	0.35
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	7	0.35
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	4	0.35
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	5	0.35
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	5	0.35
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	5	0.35
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	2	0.35
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	2	0.35
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	2	0.35
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	5	0.35
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	9	0.35
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	6	0.35
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	9	0.35
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	1	0.35
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	2	0.35
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	7	0.35
(1,70)	1:6:A:ARG:HG2	1:6:A:ARG:HG3	10	0.35
(1,68)	1:6:A:ARG:HB2	1:6:A:ARG:HG3	7	0.35
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	5	0.35
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	6	0.34
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.34
(4,32)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.34
(4,32)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.34
(4,32)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.34
(4,32)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.34
(4,32)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.34
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.34
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.34
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	5	0.34
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	5	0.34
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	5	0.34
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.34
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.34
(4,19)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.34
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.34
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	9	0.34
(3,456)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.34
(3,456)	1:10:A:GLN:HB3	1:11:A:TRP:H	1	0.34
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.34
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	4	0.34
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	10	0.34
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.34
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.34
(3,17)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.34
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	10	0.34
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	6	0.34
(2,507)	1:10:A:GLN:HB2	1:11:A:TRP:H	1	0.34
(2,507)	1:10:A:GLN:HB3	1:11:A:TRP:H	1	0.34
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	1	0.34
(2,412)	1:5:A:VAL:HG11	1:6:A:ARG:H	6	0.34
(2,412)	1:5:A:VAL:HG12	1:6:A:ARG:H	6	0.34
(2,412)	1:5:A:VAL:HG13	1:6:A:ARG:H	6	0.34
(2,412)	1:5:A:VAL:HG21	1:6:A:ARG:H	6	0.34
(2,412)	1:5:A:VAL:HG22	1:6:A:ARG:H	6	0.34
(2,412)	1:5:A:VAL:HG23	1:6:A:ARG:H	6	0.34
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	2	0.34
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	4	0.34
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	2	0.34
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	4	0.34
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	5	0.34
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	5	0.34
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD11	9	0.34
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD12	9	0.34
(2,174)	1:9:A:ILE:HA	1:9:A:ILE:HD13	9	0.34
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	10	0.34
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.34
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.34
(2,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	9	0.34
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	10	0.34
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	7	0.34
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	9	0.34
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	2	0.34
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	2	0.34
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	2	0.34
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	2	0.34
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	2	0.34
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	2	0.34
(1,556)	1:9:A:ILE:HA	1:12:A:LEU:HB3	9	0.34
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	1	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	5	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	5	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	8	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	8	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	9	0.34
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	9	0.34
(1,462)	1:6:A:ARG:HG2	1:7:A:LEU:H	2	0.34
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	7	0.34
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	7	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	5	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	5	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	5	0.34
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	5	0.34
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	5	0.34
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	5	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	5	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	5	0.34
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	5	0.34
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	5	0.34
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	5	0.34
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	5	0.34
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	2	0.34
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	2	0.34
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	2	0.34
(1,381)	1:11:A:TRP:HE1	1:21:A:ARG:HB2	9	0.34
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	1	0.34
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	6	0.34
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	1	0.34
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	3	0.34
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	9	0.34
(1,280)	1:17:A:PRO:HB2	1:17:A:PRO:HB3	10	0.34
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	5	0.34
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	7	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	2	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	5	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	7	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	8	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	9	0.34
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	10	0.34
(1,259)	1:14:A:GLN:H	1:14:A:GLN:HG2	6	0.34
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	5	0.34
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	5	0.34
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	5	0.34
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	7	0.34
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	7	0.34
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	7	0.34
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	9	0.34
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	9	0.34
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	9	0.34
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	1	0.34
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	6	0.34
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	4	0.34
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	7	0.34
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	10	0.34
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	10	0.34
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	10	0.34
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	1	0.34
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	1	0.34
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	1	0.34
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	5	0.34
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	5	0.34
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	5	0.34
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	5	0.34
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	6	0.34
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	5	0.34
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	1	0.34
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	3	0.34
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	4	0.34
(1,13)	1:3:A:GLU:H	1:4:A:ALA:H	2	0.34
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	4	0.33
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	10	0.33
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	5	0.33
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	5	0.33
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	5	0.33
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	5	0.33
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	5	0.33
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	5	0.33
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	5	0.33
(4,37)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	5	0.33
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	9	0.33
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	9	0.33
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	9	0.33
(4,32)	1:5:A:VAL:HG11	1:6:A:ARG:H	1	0.33
(4,32)	1:5:A:VAL:HG12	1:6:A:ARG:H	1	0.33
(4,32)	1:5:A:VAL:HG13	1:6:A:ARG:H	1	0.33
(4,32)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.33
(4,32)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.33
(4,32)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.33
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	0.33
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	0.33
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.33
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.33
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.33
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	3	0.33
(3,200)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.33
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.33
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.33
(3,165)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.33
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	1	0.33
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	5	0.33
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	1	0.33
(3,15)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.33
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	4	0.33
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	10	0.33
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	5	0.33
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	5	0.33
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	5	0.33
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	5	0.33
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	5	0.33
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	5	0.33
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	5	0.33
(2,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	5	0.33
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	9	0.33
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	9	0.33
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	9	0.33
(2,412)	1:5:A:VAL:HG11	1:6:A:ARG:H	1	0.33
(2,412)	1:5:A:VAL:HG12	1:6:A:ARG:H	1	0.33
(2,412)	1:5:A:VAL:HG13	1:6:A:ARG:H	1	0.33
(2,412)	1:5:A:VAL:HG21	1:6:A:ARG:H	1	0.33
(2,412)	1:5:A:VAL:HG22	1:6:A:ARG:H	1	0.33
(2,412)	1:5:A:VAL:HG23	1:6:A:ARG:H	1	0.33
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	8	0.33
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	3	0.33
(2,224)	1:12:A:LEU:H	1:12:A:LEU:HG	1	0.33
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	10	0.33
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	10	0.33
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	10	0.33
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	10	0.33
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	5	0.33
(2,184)	1:9:A:ILE:H	1:9:A:ILE:HG13	8	0.33
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	8	0.33
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	1	0.33
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	5	0.33
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	1	0.33
(2,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	2	0.33
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	3	0.33
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	3	0.33
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	3	0.33
(1,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	5	0.33
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	9	0.33
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	2	0.33
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	2	0.33
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	2	0.33
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	2	0.33
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	2	0.33
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	2	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	2	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	2	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	6	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	6	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	7	0.33
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	7	0.33
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	5	0.33
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	5	0.33
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	5	0.33
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	10	0.33
(1,335)	1:24:A:PRO:HB2	1:24:A:PRO:HD2	5	0.33
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	3	0.33
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	3	0.33
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	3	0.33
(1,274)	1:16:A:GLY:H	1:16:A:GLY:HA3	3	0.33
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	1	0.33
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:14:A:GLN:HG2	1:14:A:GLN:HG3	4	0.33
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	6	0.33
(1,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	6	0.33
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	6	0.33
(1,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	6	0.33
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD21	6	0.33
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD22	6	0.33
(1,230)	1:12:A:LEU:HB3	1:12:A:LEU:HD23	6	0.33
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	3	0.33
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	3	0.33
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	3	0.33
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	6	0.33
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	6	0.33
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	6	0.33
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	7	0.33
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	3	0.33
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	3	0.33
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	3	0.33
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	3	0.33
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	6	0.33
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	6	0.33
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	6	0.33
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	6	0.33
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	1	0.33
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	2	0.33
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	5	0.33
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	1	0.33
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	3	0.33
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	10	0.33
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	2	0.32
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	3	0.32
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	3	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	5	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	5	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	5	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	10	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	10	0.32
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	10	0.32
(4,32)	1:5:A:VAL:HG11	1:6:A:ARG:H	2	0.32
(4,32)	1:5:A:VAL:HG12	1:6:A:ARG:H	2	0.32
(4,32)	1:5:A:VAL:HG13	1:6:A:ARG:H	2	0.32
(4,32)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.32
(4,32)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.32
(4,27)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.32
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	0.32
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	3	0.32
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	3	0.32
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	1	0.32
(4,2)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.32
(3,416)	1:12:A:LEU:HG	1:13:A:LYS:H	2	0.32
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	1	0.32
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	1	0.32
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.32
(3,282)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.32
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.32
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.32
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.32
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.32
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	8	0.32
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	2	0.32
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	3	0.32
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	3	0.32
(2,460)	1:12:A:LEU:HG	1:13:A:LYS:H	2	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	5	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	5	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	5	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	10	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	10	0.32
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	10	0.32
(2,412)	1:5:A:VAL:HG11	1:6:A:ARG:H	2	0.32
(2,412)	1:5:A:VAL:HG12	1:6:A:ARG:H	2	0.32
(2,412)	1:5:A:VAL:HG13	1:6:A:ARG:H	2	0.32
(2,412)	1:5:A:VAL:HG21	1:6:A:ARG:H	2	0.32
(2,412)	1:5:A:VAL:HG22	1:6:A:ARG:H	2	0.32
(2,412)	1:5:A:VAL:HG23	1:6:A:ARG:H	2	0.32
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	1	0.32
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	1	0.32
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	6	0.32
(2,320)	1:22:A:PRO:HB3	1:22:A:PRO:HD2	10	0.32
(2,307)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	3	0.32
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	8	0.32
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	8	0.32
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	3	0.32
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	3	0.32
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	3	0.32
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	1	0.32
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	8	0.32
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	1	0.32
(2,11)	1:3:A:GLU:HB2	1:3:A:GLU:HG2	5	0.32
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	10	0.32
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	10	0.32
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	10	0.32
(1,553)	1:10:A:GLN:HA	1:13:A:LYS:HB2	5	0.32
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	8	0.32
(1,516)	1:16:A:GLY:HA2	1:17:A:PRO:HD3	4	0.32
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	1	0.32
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	1	0.32
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	1	0.32
(1,514)	1:7:A:LEU:HD11	1:10:A:GLN:HG3	2	0.32
(1,514)	1:7:A:LEU:HD12	1:10:A:GLN:HG3	2	0.32
(1,514)	1:7:A:LEU:HD13	1:10:A:GLN:HG3	2	0.32
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	1	0.32
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	1	0.32
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG2	4	0.32
(1,494)	1:17:A:PRO:HD3	1:17:A:PRO:HG3	4	0.32
(1,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	8	0.32
(1,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	8	0.32
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	6	0.32
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	8	0.32
(1,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	8	0.32
(1,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	8	0.32
(1,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	8	0.32
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	6	0.32
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	5	0.32
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	5	0.32
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	5	0.32
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	1	0.32
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	1	0.32
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	1	0.32
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	1	0.32
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	9	0.32
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	9	0.32
(1,229)	1:12:A:LEU:HB2	1:12:A:LEU:HG	6	0.32
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	10	0.32
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	10	0.32
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	5	0.32
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	5	0.32
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	10	0.32
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	4	0.32
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	4	0.32
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	4	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	4	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	4	0.32
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	9	0.32
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	9	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	9	0.32
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	9	0.32
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	1	0.32
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	1	0.32
(1,88)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.32
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	2	0.32
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	4	0.32
(1,1)	1:3:A:GLU:H	1:3:A:GLU:HA	8	0.32
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.31
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.31
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	5	0.31
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.31
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.31
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.31
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.31
(3,417)	1:12:A:LEU:HB2	1:13:A:LYS:H	1	0.31
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.31
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	1	0.31
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	2	0.31
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	4	0.31
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.31
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	2	0.31
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	9	0.31
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	9	0.31
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	5	0.31
(2,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	1	0.31
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	7	0.31
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	1	0.31
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	2	0.31
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	7	0.31
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	7	0.31
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	7	0.31
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	9	0.31
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.31
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	2	0.31
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	5	0.31
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	5	0.31
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	10	0.31
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	10	0.31
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	3	0.31
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	3	0.31
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	3	0.31
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	3	0.31
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	3	0.31
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	3	0.31
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	7	0.31
(1,462)	1:6:A:ARG:HG2	1:7:A:LEU:H	1	0.31
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	7	0.31
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	3	0.31
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	10	0.31
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	1	0.31
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	1	0.31
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	3	0.31
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	3	0.31
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	7	0.31
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	7	0.31
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	5	0.31
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	5	0.31
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	4	0.31
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	8	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	2	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	2	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	3	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	3	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	6	0.31
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	6	0.31
(1,268)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	1	0.31
(1,268)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	1	0.31
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	6	0.31
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	6	0.31
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	4	0.31
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	4	0.31
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	4	0.31
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	2	0.31
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	6	0.31
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	10	0.31
(1,200)	1:11:A:TRP:H	1:11:A:TRP:HB3	3	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB2	1	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB3	1	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB2	2	0.31
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB3	2	0.31
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	2	0.31
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	3	0.31
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	8	0.31
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	8	0.31
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	5	0.31
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	5	0.31
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	8	0.31
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	10	0.31
(1,74)	1:7:A:LEU:HA	1:7:A:LEU:HB2	7	0.31
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	8	0.31
(1,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	6	0.31
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	3	0.3
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.3
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	3	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	3	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	3	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	4	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	4	0.3
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	4	0.3
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	7	0.3
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	7	0.3
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	7	0.3
(4,32)	1:5:A:VAL:HG11	1:6:A:ARG:H	5	0.3
(4,32)	1:5:A:VAL:HG12	1:6:A:ARG:H	5	0.3
(4,32)	1:5:A:VAL:HG13	1:6:A:ARG:H	5	0.3
(4,32)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.3
(4,32)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.3
(4,32)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.3
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.3
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.3
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	3	0.3
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	3	0.3
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	6	0.3
(3,416)	1:12:A:LEU:HG	1:13:A:LYS:H	6	0.3
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	5	0.3
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	10	0.3
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	8	0.3
(3,160)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.3
(3,160)	1:9:A:ILE:HB	1:9:A:ILE:HD12	8	0.3
(3,160)	1:9:A:ILE:HB	1:9:A:ILE:HD13	8	0.3
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	10	0.3
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	3	0.3
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	5	0.3
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	5	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	3	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	3	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	3	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	4	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	4	0.3
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	4	0.3
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	3	0.3
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	3	0.3
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	6	0.3
(2,460)	1:12:A:LEU:HG	1:13:A:LYS:H	6	0.3
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	7	0.3
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	7	0.3
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	7	0.3
(2,412)	1:5:A:VAL:HG11	1:6:A:ARG:H	5	0.3
(2,412)	1:5:A:VAL:HG12	1:6:A:ARG:H	5	0.3
(2,412)	1:5:A:VAL:HG13	1:6:A:ARG:H	5	0.3
(2,412)	1:5:A:VAL:HG21	1:6:A:ARG:H	5	0.3
(2,412)	1:5:A:VAL:HG22	1:6:A:ARG:H	5	0.3
(2,412)	1:5:A:VAL:HG23	1:6:A:ARG:H	5	0.3
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	5	0.3
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	10	0.3
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	8	0.3
(2,179)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.3
(2,179)	1:9:A:ILE:HB	1:9:A:ILE:HD12	8	0.3
(2,179)	1:9:A:ILE:HB	1:9:A:ILE:HD13	8	0.3
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	8	0.3
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:7:A:LEU:H	1:7:A:LEU:HG	4	0.3
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	10	0.3
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG11	1:8:A:TYR:HD2	2	0.3
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG12	1:8:A:TYR:HD2	2	0.3
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG13	1:8:A:TYR:HD2	2	0.3
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG21	1:8:A:TYR:HD2	2	0.3
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG22	1:8:A:TYR:HD2	2	0.3
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD1	2	0.3
(1,445)	1:5:A:VAL:HG23	1:8:A:TYR:HD2	2	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	3	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	3	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	3	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	3	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	3	0.3
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	3	0.3
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	3	0.3
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	5	0.3
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	5	0.3
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	9	0.3
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	3	0.3
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	1	0.3
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	7	0.3
(1,287)	1:18:A:SER:H	1:18:A:SER:HB2	1	0.3
(1,287)	1:18:A:SER:H	1:18:A:SER:HB3	1	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	5	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	5	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	7	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	7	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	8	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	8	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	10	0.3
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	10	0.3
(1,268)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	2	0.3
(1,268)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	2	0.3
(1,258)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	8	0.3
(1,257)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	2	0.3
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	10	0.3
(1,229)	1:12:A:LEU:HB2	1:12:A:LEU:HG	4	0.3
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	8	0.3
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	8	0.3
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	8	0.3
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	4	0.3
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	4	0.3
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	4	0.3
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	2	0.3
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	7	0.3
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	7	0.3
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	7	0.3
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	9	0.3
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	2	0.3
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	2	0.3
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	2	0.3
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	2	0.3
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	2	0.3
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	2	0.3
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	8	0.3
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	8	0.3
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	8	0.3
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	8	0.3
(1,130)	1:16:A:GLY:H	1:16:A:GLY:HA2	1	0.3
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	6	0.3
(1,38)	1:6:A:ARG:HD3	1:6:A:ARG:HE	2	0.3
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	5	0.29
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.29
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.29
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	2	0.29
(4,47)	1:24:A:PRO:HD2	1:25:A:SER:HA	3	0.29
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.29
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.29
(3,416)	1:12:A:LEU:HG	1:13:A:LYS:H	4	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	7	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	7	0.29
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	7	0.29
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	7	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	7	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	7	0.29
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	7	0.29
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.29
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	6	0.29
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	7	0.29
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	10	0.29
(3,186)	1:10:A:GLN:H	1:10:A:GLN:HE22	5	0.29
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	2	0.29
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	1	0.29
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	5	0.29
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	6	0.29
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	6	0.29
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	2	0.29
(2,485)	1:24:A:PRO:HD2	1:25:A:SER:HA	3	0.29
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	5	0.29
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	5	0.29
(2,460)	1:12:A:LEU:HG	1:13:A:LYS:H	4	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	7	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	7	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	7	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	7	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	7	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	7	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	7	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	7	0.29
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	7	0.29
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	7	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	7	0.29
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	7	0.29
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	2	0.29
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	6	0.29
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	7	0.29
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	10	0.29
(2,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	5	0.29
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	2	0.29
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	1	0.29
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	3	0.29
(1,460)	1:12:A:LEU:HG	1:13:A:LYS:H	10	0.29
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	1	0.29
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	1	0.29
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	10	0.29
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	10	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	2	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	4	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	7	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	8	0.29
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	9	0.29
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	6	0.29
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	6	0.29
(1,268)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	10	0.29
(1,268)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	10	0.29
(1,254)	1:14:A:GLN:HA	1:14:A:GLN:HE21	1	0.29
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	7	0.29
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	7	0.29
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	9	0.29
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	9	0.29
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	10	0.29
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	2	0.29
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	2	0.29
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	2	0.29
(1,189)	1:19:A:SER:HG	1:21:A:ARG:H	9	0.29
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	9	0.29
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	6	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	1	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	1	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	3	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	3	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	4	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	4	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	5	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	7	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	7	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	9	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	9	0.29
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	10	0.29
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	10	0.29
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	10	0.29
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	10	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	5	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	5	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	5	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	6	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	6	0.29
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	6	0.29
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	6	0.29
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.29
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	9	0.29
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	9	0.28
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	9	0.28
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	1	0.28
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	1	0.28
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	1	0.28
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD21	9	0.28
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD22	9	0.28
(4,22)	1:12:A:LEU:HA	1:12:A:LEU:HD23	9	0.28
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	4	0.28
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	4	0.28
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	4	0.28
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	6	0.28
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	6	0.28
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	6	0.28
(3,452)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	5	0.28
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.28
(3,282)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.28
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	4	0.28
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	6	0.28
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	6	0.28
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	6	0.28
(2,501)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	5	0.28
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	9	0.28
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	1	0.28
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	1	0.28
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	1	0.28
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	1	0.28
(2,307)	1:21:A:ARG:HB3	1:21:A:ARG:HG3	10	0.28
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	9	0.28
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	9	0.28
(2,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	9	0.28
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	4	0.28
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	4	0.28
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	4	0.28
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	4	0.28
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	4	0.28
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	4	0.28
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	4	0.28
(1,554)	1:9:A:ILE:HA	1:12:A:LEU:HG	1	0.28
(1,551)	1:7:A:LEU:HA	1:10:A:GLN:HG3	9	0.28
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	4	0.28
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	4	0.28
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	7	0.28
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	7	0.28
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	2	0.28
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	1	0.28
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	5	0.28
(1,304)	1:21:A:ARG:HB2	1:21:A:ARG:HB3	6	0.28
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	4	0.28
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	4	0.28
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	9	0.28
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	9	0.28
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	2	0.28
(1,268)	1:14:A:GLN:HB2	1:14:A:GLN:HG3	6	0.28
(1,268)	1:14:A:GLN:HB3	1:14:A:GLN:HG3	6	0.28
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	8	0.28
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	8	0.28
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	3	0.28
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	1	0.28
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	1	0.28
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	1	0.28
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	3	0.28
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	3	0.28
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	3	0.28
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	10	0.28
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	10	0.28
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD21	2	0.28
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD22	2	0.28
(1,216)	1:12:A:LEU:HA	1:12:A:LEU:HD23	2	0.28
(1,151)	1:24:A:PRO:HA	1:24:A:PRO:HB3	8	0.28
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	1	0.28
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	3	0.28
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	9	0.28
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	9	0.28
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	9	0.28
(1,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	3	0.28
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	10	0.28
(1,4)	1:3:A:GLU:HA	1:3:A:GLU:HG3	8	0.28
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	7	0.28
(4,44)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	6	0.27
(4,44)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	6	0.27
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	4	0.27
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	4	0.27
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	4	0.27
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	2	0.27
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	8	0.27
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	7	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	3	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	3	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	3	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	10	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	10	0.27
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	10	0.27
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.27
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	3	0.27
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	3	0.27
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	3	0.27
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE2	1	0.27
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE3	1	0.27
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	10	0.27
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	10	0.27
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	4	0.27
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	4	0.27
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	4	0.27
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	6	0.27
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,311)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	9	0.27
(3,216)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	0.27
(3,216)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	1	0.27
(3,216)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.27
(3,175)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.27
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.27
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.27
(3,81)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.27
(3,53)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	0.27
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	4	0.27
(3,43)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.27
(3,17)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.27
(3,17)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.27
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	3	0.27
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE2	1	0.27
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE3	1	0.27
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	10	0.27
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	10	0.27
(2,452)	1:8:A:TYR:HD1	1:12:A:LEU:HB2	6	0.27
(2,452)	1:8:A:TYR:HD2	1:12:A:LEU:HB2	6	0.27
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	4	0.27
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	4	0.27
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	4	0.27
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	4	0.27
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	4	0.27
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	4	0.27
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	6	0.27
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	2	0.27
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	8	0.27
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	7	0.27
(2,338)	1:24:A:PRO:HB3	1:24:A:PRO:HD3	9	0.27
(2,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE2	1	0.27
(2,241)	1:13:A:LYS:HB2	1:13:A:LYS:HE3	1	0.27
(2,241)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.27
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	7	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	3	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	3	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	3	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	10	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	10	0.27
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	10	0.27
(2,195)	1:10:A:GLN:H	1:10:A:GLN:HG3	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	8	0.27
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	3	0.27
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	3	0.27
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	3	0.27
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	5	0.27
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	6	0.27
(2,90)	1:7:A:LEU:H	1:7:A:LEU:HB2	9	0.27
(2,57)	1:6:A:ARG:HB2	1:6:A:ARG:HD3	9	0.27
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	4	0.27
(2,47)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.27
(2,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	5	0.27
(2,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	7	0.27
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	3	0.27
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	9	0.27
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	9	0.27
(1,490)	1:6:A:ARG:HA	1:9:A:ILE:HB	4	0.27
(1,460)	1:12:A:LEU:HG	1:13:A:LYS:H	3	0.27
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	3	0.27
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	3	0.27
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	3	0.27
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	3	0.27
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	3	0.27
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	3	0.27
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	7	0.27
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	7	0.27
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	7	0.27
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	2	0.27
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	2	0.27
(1,350)	1:23:A:PRO:HA	1:24:A:PRO:HD2	10	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	1	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	3	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	4	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	5	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	6	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	7	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	8	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	9	0.27
(1,349)	1:24:A:PRO:HD2	1:24:A:PRO:HD3	10	0.27
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG2	4	0.27
(1,282)	1:17:A:PRO:HD2	1:17:A:PRO:HG3	4	0.27
(1,229)	1:12:A:LEU:HB2	1:12:A:LEU:HG	2	0.27
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	2	0.27
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	2	0.27
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	4	0.27
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	4	0.27
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	4	0.27
(1,218)	1:12:A:LEU:HD21	1:12:A:LEU:HG	6	0.27
(1,218)	1:12:A:LEU:HD22	1:12:A:LEU:HG	6	0.27
(1,218)	1:12:A:LEU:HD23	1:12:A:LEU:HG	6	0.27
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	5	0.27
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	5	0.27
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	5	0.27
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	7	0.27
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	7	0.27
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	7	0.27
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	9	0.27
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	9	0.27
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	9	0.27
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	5	0.27
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	10	0.27
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	9	0.27
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	9	0.27
(1,146)	1:23:A:PRO:HD2	1:23:A:PRO:HG2	6	0.27
(1,146)	1:23:A:PRO:HD3	1:23:A:PRO:HG2	6	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	3	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	3	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	7	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	7	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	8	0.27
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	8	0.27
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	7	0.27
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	3	0.27
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	3	0.27
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	3	0.27
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.27
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	7	0.26
(4,68)	1:11:A:TRP:HZ3	1:12:A:LEU:H	9	0.26
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	1	0.26
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	1	0.26
(4,29)	1:24:A:PRO:HA	1:25:A:SER:H	8	0.26
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	4	0.26
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	6	0.26
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	9	0.26
(4,4)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.26
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	3	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	9	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	9	0.26
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	9	0.26
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	9	0.26
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	9	0.26
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.26
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.26
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.26
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.26
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	9	0.26
(3,141)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.26
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	2	0.26
(3,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	6	0.26
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	7	0.26
(2,562)	1:11:A:TRP:HZ3	1:12:A:LEU:H	9	0.26
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	1	0.26
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	1	0.26
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	3	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	9	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	9	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	9	0.26
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	9	0.26
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	9	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	9	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	9	0.26
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	9	0.26
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	9	0.26
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	9	0.26
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	9	0.26
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	9	0.26
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	1	0.26
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	8	0.26
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	10	0.26
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	10	0.26
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	9	0.26
(2,363)	1:24:A:PRO:HA	1:25:A:SER:H	8	0.26
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	4	0.26
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	6	0.26
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	5	0.26
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	9	0.26
(2,158)	1:11:A:TRP:HZ2	1:17:A:PRO:HD2	4	0.26
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	2	0.26
(2,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.26
(2,9)	1:3:A:GLU:HB3	1:3:A:GLU:HG2	6	0.26
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	10	0.26
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	1	0.26
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	1	0.26
(1,476)	1:13:A:LYS:HB2	1:14:A:GLN:H	4	0.26
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	2	0.26
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG2	4	0.26
(1,453)	1:10:A:GLN:HE22	1:13:A:LYS:HG3	4	0.26
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	8	0.26
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	8	0.26
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	8	0.26
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	8	0.26
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	8	0.26
(1,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	8	0.26
(1,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	8	0.26
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	5	0.26
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	8	0.26
(1,303)	1:21:A:ARG:HD2	1:21:A:ARG:HG3	2	0.26
(1,303)	1:21:A:ARG:HD3	1:21:A:ARG:HG3	2	0.26
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	8	0.26
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	8	0.26
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	3	0.26
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	8	0.26
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	8	0.26
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	8	0.26
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	8	0.26
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	8	0.26
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	8	0.26
(1,197)	1:10:A:GLN:HE21	1:10:A:GLN:HG3	6	0.26
(1,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	4	0.26
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	9	0.26
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	8	0.26
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	7	0.26
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	2	0.26
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	5	0.26
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	1	0.26
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.25
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.25
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	9	0.25
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	9	0.25
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	9	0.25
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	7	0.25
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	7	0.25
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	3	0.25
(4,25)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	7	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	7	0.25
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	7	0.25
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.25
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.25
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	0.25
(3,493)	1:9:A:ILE:HG21	1:12:A:LEU:HG	6	0.25
(3,493)	1:9:A:ILE:HG22	1:12:A:LEU:HG	6	0.25
(3,493)	1:9:A:ILE:HG23	1:12:A:LEU:HG	6	0.25
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	4	0.25
(3,437)	1:13:A:LYS:H	1:14:A:GLN:HG2	1	0.25
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	10	0.25
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	10	0.25
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.25
(3,361)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.25
(3,343)	1:19:A:SER:H	1:20:A:GLY:HA3	8	0.25
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	1	0.25
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	1	0.25
(3,207)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	1	0.25
(3,48)	1:6:A:ARG:HB2	1:6:A:ARG:HE	3	0.25
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	5	0.25
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	7	0.25
(2,560)	1:9:A:ILE:HG21	1:12:A:LEU:HG	6	0.25
(2,560)	1:9:A:ILE:HG22	1:12:A:LEU:HG	6	0.25
(2,560)	1:9:A:ILE:HG23	1:12:A:LEU:HG	6	0.25
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	4	0.25
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	3	0.25
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	3	0.25
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	9	0.25
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	9	0.25
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	9	0.25
(2,483)	1:13:A:LYS:H	1:14:A:GLN:HG2	1	0.25
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	7	0.25
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	7	0.25
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	10	0.25
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	10	0.25
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	5	0.25
(2,391)	1:11:A:TRP:HZ2	1:17:A:PRO:HB2	3	0.25
(2,373)	1:19:A:SER:H	1:20:A:GLY:HA3	8	0.25
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	3	0.25
(2,236)	1:12:A:LEU:H	1:12:A:LEU:HB2	10	0.25
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD11	1	0.25
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD12	1	0.25
(2,231)	1:12:A:LEU:HB3	1:12:A:LEU:HD13	1	0.25
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	7	0.25
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	7	0.25
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	3	0.25
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	3	0.25
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	3	0.25
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	7	0.25
(2,52)	1:6:A:ARG:HB2	1:6:A:ARG:HE	3	0.25
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	5	0.25
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	7	0.25
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	6	0.25
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	6	0.25
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	6	0.25
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	6	0.25
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	6	0.25
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	6	0.25
(1,426)	1:5:A:VAL:HG11	1:9:A:ILE:HG13	4	0.25
(1,426)	1:5:A:VAL:HG12	1:9:A:ILE:HG13	4	0.25
(1,426)	1:5:A:VAL:HG13	1:9:A:ILE:HG13	4	0.25
(1,426)	1:5:A:VAL:HG21	1:9:A:ILE:HG13	4	0.25
(1,426)	1:5:A:VAL:HG22	1:9:A:ILE:HG13	4	0.25
(1,426)	1:5:A:VAL:HG23	1:9:A:ILE:HG13	4	0.25
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	3	0.25
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	5	0.25
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	8	0.25
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	10	0.25
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	5	0.25
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	2	0.25
(1,315)	1:21:A:ARG:H	1:21:A:ARG:HG3	3	0.25
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	6	0.25
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	1	0.25
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	1	0.25
(1,177)	1:9:A:ILE:HB	1:9:A:ILE:HG12	8	0.25
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	2	0.25
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	8	0.25
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	8	0.25
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	2	0.25
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	2	0.25
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	9	0.25
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	9	0.25
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	1	0.25
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	4	0.25
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	4	0.25
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	5	0.25
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	1	0.25
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.25
(1,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	6	0.25
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	2	0.25
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	10	0.25
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	5	0.24
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	5	0.24
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	5	0.24
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	1	0.24
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	1	0.24
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	1	0.24
(4,34)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	2	0.24
(4,34)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	2	0.24
(4,34)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	2	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	5	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.24
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.24
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.24
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	0.24
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.24
(4,3)	1:3:A:GLU:H	1:3:A:GLU:HB2	6	0.24
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.24
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.24
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	3	0.24
(3,441)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.24
(3,399)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.24
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.24
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.24
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	10	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	10	0.24
(3,393)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	10	0.24
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	10	0.24
(3,393)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	10	0.24
(3,393)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	10	0.24
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.24
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.24
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.24
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	3	0.24
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	3	0.24
(3,391)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	3	0.24
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	7	0.24
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	9	0.24
(3,163)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	8	0.24
(3,163)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	8	0.24
(3,163)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	8	0.24
(3,17)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.24
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	3	0.24
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	5	0.24
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	5	0.24
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	5	0.24
(2,488)	1:8:A:TYR:HA	1:24:A:PRO:HG3	8	0.24
(2,438)	1:11:A:TRP:HE3	1:12:A:LEU:HG	8	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG11	10	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG12	10	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG13	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG11	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG12	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG13	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG11	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG12	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG13	10	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG21	10	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG22	10	0.24
(2,429)	1:4:A:ALA:HB1	1:5:A:VAL:HG23	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG21	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG22	10	0.24
(2,429)	1:4:A:ALA:HB2	1:5:A:VAL:HG23	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG21	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG22	10	0.24
(2,429)	1:4:A:ALA:HB3	1:5:A:VAL:HG23	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	8	0.24
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	8	0.24
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	8	0.24
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	3	0.24
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	3	0.24
(2,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	3	0.24
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	1	0.24
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	1	0.24
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	1	0.24
(2,422)	1:7:A:LEU:HD21	1:10:A:GLN:HG3	2	0.24
(2,422)	1:7:A:LEU:HD22	1:10:A:GLN:HG3	2	0.24
(2,422)	1:7:A:LEU:HD23	1:10:A:GLN:HG3	2	0.24
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	7	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	5	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	5	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	5	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	9	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	9	0.24
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	9	0.24
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	9	0.24
(2,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	8	0.24
(2,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	8	0.24
(2,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	8	0.24
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	1	0.24
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	3	0.24
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	5	0.24
(2,20)	1:3:A:GLU:H	1:3:A:GLU:HG2	1	0.24
(2,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	6	0.24
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	7	0.24
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	9	0.24
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	8	0.24
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	8	0.24
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	8	0.24
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	8	0.24
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	8	0.24
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	8	0.24
(1,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	5	0.24
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	7	0.24
(1,521)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	6	0.24
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	6	0.24
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	6	0.24
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	4	0.24
(1,367)	1:8:A:TYR:HA	1:8:A:TYR:HD1	8	0.24
(1,367)	1:8:A:TYR:HA	1:8:A:TYR:HD2	8	0.24
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	1	0.24
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	2	0.24
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	7	0.24
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	4	0.24
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	1	0.24
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	3	0.24
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	10	0.24
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	7	0.24
(1,302)	1:21:A:ARG:HD2	1:21:A:ARG:HG2	10	0.24
(1,302)	1:21:A:ARG:HD3	1:21:A:ARG:HG2	10	0.24
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	5	0.24
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	5	0.24
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	9	0.24
(1,191)	1:10:A:GLN:HA	1:10:A:GLN:HG2	3	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG21	8	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG22	8	0.24
(1,173)	1:9:A:ILE:HA	1:9:A:ILE:HG23	8	0.24
(1,166)	1:8:A:TYR:H	1:9:A:ILE:H	6	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	1	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	1	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	2	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	2	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	3	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	3	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	4	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	4	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	5	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	5	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	7	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	7	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	9	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	9	0.24
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	10	0.24
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	10	0.24
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	1	0.24
(1,62)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	9	0.24
(1,17)	1:3:A:GLU:H	1:3:A:GLU:HB3	8	0.24
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	5	0.23
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	5	0.23
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	0.23
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	0.23
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	0.23
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	1	0.23
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	1	0.23
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	1	0.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	2	0.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	2	0.23
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	2	0.23
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	7	0.23
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	9	0.23
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.23
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.23
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.23
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.23
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	8	0.23
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	4	0.23
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.23
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.23
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.23
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.23
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.23
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	7	0.23
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	5	0.23
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	5	0.23
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	5	0.23
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	4	0.23
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	1	0.23
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	1	0.23
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	1	0.23
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	1	0.23
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	1	0.23
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	1	0.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	2	0.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	2	0.23
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	2	0.23
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	7	0.23
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	9	0.23
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	5	0.23
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	5	0.23
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.23
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	6	0.23
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	4	0.23
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	4	0.23
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	7	0.23
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	7	0.23
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	7	0.23
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	8	0.23
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	3	0.23
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	3	0.23
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	3	0.23
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	3	0.23
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	3	0.23
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	3	0.23
(1,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	4	0.23
(1,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	4	0.23
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD21	2	0.23
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD22	2	0.23
(1,449)	1:8:A:TYR:HE1	1:12:A:LEU:HD23	2	0.23
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD21	2	0.23
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD22	2	0.23
(1,449)	1:8:A:TYR:HE2	1:12:A:LEU:HD23	2	0.23
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	2	0.23
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	2	0.23
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	2	0.23
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	2	0.23
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	2	0.23
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	2	0.23
(1,434)	1:13:A:LYS:HG2	1:14:A:GLN:HA	8	0.23
(1,434)	1:13:A:LYS:HG3	1:14:A:GLN:HA	8	0.23
(1,357)	1:11:A:TRP:HE1	1:17:A:PRO:HA	1	0.23
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	4	0.23
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	6	0.23
(1,348)	1:24:A:PRO:HG2	1:24:A:PRO:HG3	9	0.23
(1,345)	1:24:A:PRO:HB2	1:24:A:PRO:HG2	6	0.23
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	2	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	2	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	3	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	4	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	5	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	6	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	8	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	9	0.23
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	10	0.23
(1,217)	1:12:A:LEU:HD11	1:12:A:LEU:HG	1	0.23
(1,217)	1:12:A:LEU:HD12	1:12:A:LEU:HG	1	0.23
(1,217)	1:12:A:LEU:HD13	1:12:A:LEU:HG	1	0.23
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	6	0.23
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	6	0.23
(1,147)	1:23:A:PRO:HD2	1:23:A:PRO:HG3	6	0.23
(1,147)	1:23:A:PRO:HD3	1:23:A:PRO:HG3	6	0.23
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD2	10	0.23
(1,145)	1:22:A:PRO:HG2	1:23:A:PRO:HD3	10	0.23
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD2	10	0.23
(1,145)	1:22:A:PRO:HG3	1:23:A:PRO:HD3	10	0.23
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	6	0.23
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	6	0.23
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	3	0.23
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	4	0.23
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	5	0.23
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	8	0.23
(1,69)	1:6:A:ARG:HB3	1:6:A:ARG:HG3	2	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	1	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	2	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	3	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	4	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	6	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	7	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	8	0.23
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	10	0.23
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	10	0.23
(1,27)	1:4:A:ALA:H	1:5:A:VAL:H	7	0.23
(1,21)	1:3:A:GLU:HB3	1:4:A:ALA:H	2	0.23
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	1	0.23
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	8	0.23
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.22
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.22
(4,46)	1:8:A:TYR:HE1	1:12:A:LEU:HG	10	0.22
(4,46)	1:8:A:TYR:HE2	1:12:A:LEU:HG	10	0.22
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD11	3	0.22
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD12	3	0.22
(4,31)	1:4:A:ALA:H	1:9:A:ILE:HD13	3	0.22
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.22
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	1	0.22
(4,1)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.22
(3,493)	1:9:A:ILE:HG21	1:12:A:LEU:HG	4	0.22
(3,493)	1:9:A:ILE:HG22	1:12:A:LEU:HG	4	0.22
(3,493)	1:9:A:ILE:HG23	1:12:A:LEU:HG	4	0.22
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	1	0.22
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	1	0.22
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	1	0.22
(3,431)	1:13:A:LYS:HB3	1:14:A:GLN:H	1	0.22
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.22
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.22
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.22
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.22
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.22
(3,43)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.22
(2,560)	1:9:A:ILE:HG21	1:12:A:LEU:HG	4	0.22
(2,560)	1:9:A:ILE:HG22	1:12:A:LEU:HG	4	0.22
(2,560)	1:9:A:ILE:HG23	1:12:A:LEU:HG	4	0.22
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	5	0.22
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	7	0.22
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	1	0.22
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	1	0.22
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	1	0.22
(2,480)	1:8:A:TYR:HE1	1:12:A:LEU:HG	10	0.22
(2,480)	1:8:A:TYR:HE2	1:12:A:LEU:HG	10	0.22
(2,476)	1:13:A:LYS:HB3	1:14:A:GLN:H	1	0.22
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD11	3	0.22
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD12	3	0.22
(2,406)	1:4:A:ALA:H	1:9:A:ILE:HD13	3	0.22
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	5	0.22
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	2	0.22
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	10	0.22
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	1	0.22
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	1	0.22
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	2	0.22
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	2	0.22
(2,47)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.22
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	1	0.22
(2,8)	1:3:A:GLU:HB3	1:3:A:GLU:HG3	5	0.22
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	1	0.22
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	1	0.22
(1,484)	1:8:A:TYR:HE1	1:23:A:PRO:HB2	1	0.22
(1,484)	1:8:A:TYR:HE2	1:23:A:PRO:HB2	1	0.22
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	2	0.22
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	4	0.22
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	3	0.22
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	3	0.22
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	5	0.22
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	10	0.22
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	1	0.22
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	1	0.22
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	7	0.22
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	9	0.22
(1,299)	1:21:A:ARG:HA	1:21:A:ARG:HG3	3	0.22
(1,293)	1:20:A:GLY:HA2	1:20:A:GLY:HA3	1	0.22
(1,235)	1:12:A:LEU:H	1:12:A:LEU:HB3	8	0.22
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD2	4	0.22
(1,141)	1:22:A:PRO:HA	1:23:A:PRO:HD3	4	0.22
(1,139)	1:21:A:ARG:HA	1:22:A:PRO:HD2	9	0.22
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	2	0.22
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	6	0.22
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	7	0.22
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	1	0.22
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	1	0.22
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	1	0.22
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	1	0.22
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	2	0.22
(1,65)	1:6:A:ARG:HB2	1:6:A:ARG:HB3	9	0.22
(1,50)	1:6:A:ARG:HE	1:6:A:ARG:HG2	9	0.22
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.22
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	10	0.22
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	5	0.22
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB1	2	0.21
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB2	2	0.21
(4,39)	1:3:A:GLU:HA	1:4:A:ALA:HB3	2	0.21
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	4	0.21
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	4	0.21
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	4	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.21
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.21
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.21
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.21
(3,491)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	8	0.21
(3,491)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	8	0.21
(3,491)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	8	0.21
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	9	0.21
(3,469)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	4	0.21
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.21
(3,136)	1:24:A:PRO:HA	1:24:A:PRO:HG3	2	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.21
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.21
(2,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	8	0.21
(2,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	8	0.21
(2,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	8	0.21
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	9	0.21
(2,526)	1:11:A:TRP:HE3	1:17:A:PRO:HD2	4	0.21
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB1	2	0.21
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB2	2	0.21
(2,435)	1:3:A:GLU:HA	1:4:A:ALA:HB3	2	0.21
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	4	0.21
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	4	0.21
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	4	0.21
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	6	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	1	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	1	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	7	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	7	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	8	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	8	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	10	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	10	0.21
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.21
(2,153)	1:24:A:PRO:HA	1:24:A:PRO:HG3	2	0.21
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	3	0.21
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	3	0.21
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	5	0.21
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	5	0.21
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	9	0.21
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	9	0.21
(1,512)	1:8:A:TYR:HD1	1:24:A:PRO:HD2	8	0.21
(1,512)	1:8:A:TYR:HD2	1:24:A:PRO:HD2	8	0.21
(1,468)	1:11:A:TRP:HZ2	1:17:A:PRO:HB3	4	0.21
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	10	0.21
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	10	0.21
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	10	0.21
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	10	0.21
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	10	0.21
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	10	0.21
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	1	0.21
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	3	0.21
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	7	0.21
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	10	0.21
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	2	0.21
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	6	0.21
(1,402)	1:4:A:ALA:H	1:5:A:VAL:HB	8	0.21
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	8	0.21
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	1	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	2	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	2	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	3	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	3	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	6	0.21
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	6	0.21
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	8	0.21
(1,118)	1:20:A:GLY:H	1:20:A:GLY:HA2	10	0.21
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	2	0.21
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	2	0.21
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	2	0.21
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	10	0.21
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	10	0.21
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:6:A:ARG:HD2	1:6:A:ARG:HG2	6	0.21
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.21
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	7	0.21
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	4	0.21
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD11	3	0.2
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD12	3	0.2
(4,35)	1:5:A:VAL:HB	1:7:A:LEU:HD13	3	0.2
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	7	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.2
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.2
(3,492)	1:4:A:ALA:HB1	1:5:A:VAL:HB	2	0.2
(3,492)	1:4:A:ALA:HB2	1:5:A:VAL:HB	2	0.2
(3,492)	1:4:A:ALA:HB3	1:5:A:VAL:HB	2	0.2
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	4	0.2
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	4	0.2
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	4	0.2
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.2
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.2
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE2	2	0.2
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE3	2	0.2
(3,401)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	6	0.2
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	6	0.2
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD1	2	0.2
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD2	2	0.2
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD1	4	0.2
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD2	4	0.2
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.2
(3,190)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.2
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.2
(3,171)	1:10:A:GLN:HA	1:10:A:GLN:HG2	1	0.2
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.2
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.2
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2
(3,49)	1:5:A:VAL:H	1:6:A:ARG:HB2	10	0.2
(3,42)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.2
(3,32)	1:5:A:VAL:HA	1:6:A:ARG:H	8	0.2
(3,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,558)	1:4:A:ALA:HB1	1:5:A:VAL:HB	2	0.2
(2,558)	1:4:A:ALA:HB2	1:5:A:VAL:HB	2	0.2
(2,558)	1:4:A:ALA:HB3	1:5:A:VAL:HB	2	0.2
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	4	0.2
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	4	0.2
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	4	0.2
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	1	0.2
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	5	0.2
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE2	2	0.2
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE3	2	0.2
(2,442)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	6	0.2
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD11	3	0.2
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD12	3	0.2
(2,423)	1:5:A:VAL:HB	1:7:A:LEU:HD13	3	0.2
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	6	0.2
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	2	0.2
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	2	0.2
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	4	0.2
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	4	0.2
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	7	0.2
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	8	0.2
(2,210)	1:11:A:TRP:HB2	1:12:A:LEU:H	8	0.2
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	8	0.2
(2,191)	1:10:A:GLN:HA	1:10:A:GLN:HG2	1	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	4	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	4	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	9	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	9	0.2
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.2
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	6	0.2
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	6	0.2
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	10	0.2
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	10	0.2
(2,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	10	0.2
(2,45)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.2
(2,35)	1:5:A:VAL:HA	1:6:A:ARG:H	8	0.2
(2,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	6	0.2
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	2	0.2
(1,472)	1:16:A:GLY:HA2	1:17:A:PRO:HD2	1	0.2
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE2	10	0.2
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE2	10	0.2
(1,420)	1:9:A:ILE:HG21	1:13:A:LYS:HE3	10	0.2
(1,420)	1:9:A:ILE:HG22	1:13:A:LYS:HE3	10	0.2
(1,420)	1:9:A:ILE:HG23	1:13:A:LYS:HE3	10	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	1	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	3	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	5	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	7	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	8	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	9	0.2
(1,417)	1:17:A:PRO:HD2	1:17:A:PRO:HD3	10	0.2
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	4	0.2
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	4	0.2
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	6	0.2
(1,310)	1:21:A:ARG:HB2	1:21:A:ARG:HE	10	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	5	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	5	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	7	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	7	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	8	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	8	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	9	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	9	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	10	0.2
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	10	0.2
(1,237)	1:13:A:LYS:HA	1:13:A:LYS:HB2	1	0.2
(1,237)	1:13:A:LYS:HA	1:13:A:LYS:HB3	1	0.2
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	1	0.2
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	5	0.2
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	5	0.2
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	3	0.2
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	4	0.2
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	4	0.2
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	4	0.2
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	10	0.2
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	10	0.2
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	10	0.2
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	7	0.2
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	10	0.2
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	8	0.2
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	7	0.2
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	1	0.2
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	5	0.2
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	7	0.2
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	9	0.2
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	3	0.2
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD11	6	0.19
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD12	6	0.19
(4,48)	1:6:A:ARG:HA	1:7:A:LEU:HD13	6	0.19
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG2	3	0.19
(4,45)	1:12:A:LEU:HG	1:13:A:LYS:HG3	3	0.19
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	2	0.19
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	5	0.19
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.19
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.19
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.19
(4,16)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.19
(3,492)	1:4:A:ALA:HB1	1:5:A:VAL:HB	1	0.19
(3,492)	1:4:A:ALA:HB2	1:5:A:VAL:HB	1	0.19
(3,492)	1:4:A:ALA:HB3	1:5:A:VAL:HB	1	0.19
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.19
(3,452)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	1	0.19
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	1	0.19
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	1	0.19
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	4	0.19
(3,357)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.19
(3,357)	1:11:A:TRP:HZ2	1:16:A:GLY:HA2	4	0.19
(3,319)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.19
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.19
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.19
(3,171)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.19
(3,56)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	0.19
(3,43)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.19
(3,21)	1:3:A:GLU:HG2	1:4:A:ALA:H	9	0.19
(2,558)	1:4:A:ALA:HB1	1:5:A:VAL:HB	1	0.19
(2,558)	1:4:A:ALA:HB2	1:5:A:VAL:HB	1	0.19
(2,558)	1:4:A:ALA:HB3	1:5:A:VAL:HB	1	0.19
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	10	0.19
(2,501)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	1	0.19
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD11	6	0.19
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD12	6	0.19
(2,495)	1:6:A:ARG:HA	1:7:A:LEU:HD13	6	0.19
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	1	0.19
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG2	3	0.19
(2,473)	1:12:A:LEU:HG	1:13:A:LYS:HG3	3	0.19
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	4	0.19
(2,387)	1:11:A:TRP:HH2	1:16:A:GLY:HA2	4	0.19
(2,387)	1:11:A:TRP:HZ2	1:16:A:GLY:HA2	4	0.19
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	2	0.19
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	5	0.19
(2,347)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	2	0.19
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	1	0.19
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	7	0.19
(2,191)	1:10:A:GLN:HA	1:10:A:GLN:HG2	2	0.19
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	2	0.19
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.19
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	2	0.19
(2,138)	1:22:A:PRO:HA	1:22:A:PRO:HD3	4	0.19
(2,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	6	0.19
(2,47)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.19
(2,24)	1:3:A:GLU:HG2	1:4:A:ALA:H	9	0.19
(1,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	2	0.19
(1,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	2	0.19
(1,493)	1:17:A:PRO:HB3	1:17:A:PRO:HD3	4	0.19
(1,490)	1:6:A:ARG:HA	1:9:A:ILE:HB	1	0.19
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	6	0.19
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	6	0.19
(1,465)	1:11:A:TRP:HH2	1:23:A:PRO:HB3	8	0.19
(1,465)	1:11:A:TRP:HZ2	1:23:A:PRO:HB3	8	0.19
(1,463)	1:6:A:ARG:HG3	1:7:A:LEU:H	5	0.19
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	5	0.19
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	6	0.19
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	8	0.19
(1,418)	1:6:A:ARG:HD2	1:6:A:ARG:HD3	9	0.19
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	2	0.19
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	2	0.19
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD2	3	0.19
(1,377)	1:11:A:TRP:HE1	1:23:A:PRO:HD3	3	0.19
(1,360)	1:6:A:ARG:HA	1:9:A:ILE:H	6	0.19
(1,332)	1:23:A:PRO:HB2	1:23:A:PRO:HG2	6	0.19
(1,288)	1:18:A:SER:HB2	1:19:A:SER:H	9	0.19
(1,288)	1:18:A:SER:HB3	1:19:A:SER:H	9	0.19
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	1	0.19
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	3	0.19
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE2	10	0.19
(1,240)	1:13:A:LYS:HA	1:13:A:LYS:HE3	10	0.19
(1,205)	1:11:A:TRP:HB3	1:11:A:TRP:HD1	1	0.19
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	5	0.19
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	3	0.19
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	6	0.19
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	8	0.19
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	4	0.19
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	5	0.19
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	7	0.19
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	9	0.19
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	9	0.19
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	10	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	1	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	1	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	1	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	2	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	2	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	2	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	3	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	3	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	3	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	5	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	5	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	5	0.19
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	7	0.19
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	7	0.19
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	7	0.19
(1,54)	1:5:A:VAL:H	1:6:A:ARG:HG2	4	0.19
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	2	0.19
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	3	0.19
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	4	0.19
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	10	0.19
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	4	0.19
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.18
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	0.18
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.18
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	1	0.18
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	8	0.18
(4,26)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.18
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	0.18
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	0.18
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	1	0.18
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	1	0.18
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	1	0.18
(3,492)	1:4:A:ALA:HB1	1:5:A:VAL:HB	5	0.18
(3,492)	1:4:A:ALA:HB2	1:5:A:VAL:HB	5	0.18
(3,492)	1:4:A:ALA:HB3	1:5:A:VAL:HB	5	0.18
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	3	0.18
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	3	0.18
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	3	0.18
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	10	0.18
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD1	1	0.18
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD2	1	0.18
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.18
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.18
(3,79)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.18
(3,79)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.18
(3,79)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.18
(2,558)	1:4:A:ALA:HB1	1:5:A:VAL:HB	5	0.18
(2,558)	1:4:A:ALA:HB2	1:5:A:VAL:HB	5	0.18
(2,558)	1:4:A:ALA:HB3	1:5:A:VAL:HB	5	0.18
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	4	0.18
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	4	0.18
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	10	0.18
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	3	0.18
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	3	0.18
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	3	0.18
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	10	0.18
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	1	0.18
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	1	0.18
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	1	0.18
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	8	0.18
(2,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	10	0.18
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	4	0.18
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	7	0.18
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	5	0.18
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	5	0.18
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	5	0.18
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	1	0.18
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	1	0.18
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:7:A:LEU:H	1:7:A:LEU:HD21	8	0.18
(2,86)	1:7:A:LEU:H	1:7:A:LEU:HD22	8	0.18
(2,86)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.18
(1,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	5	0.18
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	6	0.18
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	1	0.18
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	1	0.18
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	1	0.18
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	1	0.18
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	1	0.18
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	1	0.18
(1,476)	1:13:A:LYS:HB2	1:14:A:GLN:H	2	0.18
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	7	0.18
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	7	0.18
(1,408)	1:5:A:VAL:HG11	1:9:A:ILE:H	10	0.18
(1,408)	1:5:A:VAL:HG12	1:9:A:ILE:H	10	0.18
(1,408)	1:5:A:VAL:HG13	1:9:A:ILE:H	10	0.18
(1,408)	1:5:A:VAL:HG21	1:9:A:ILE:H	10	0.18
(1,408)	1:5:A:VAL:HG22	1:9:A:ILE:H	10	0.18
(1,408)	1:5:A:VAL:HG23	1:9:A:ILE:H	10	0.18
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	7	0.18
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	8	0.18
(1,312)	1:21:A:ARG:HE	1:21:A:ARG:HG2	7	0.18
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG2	4	0.18
(1,279)	1:17:A:PRO:HB2	1:17:A:PRO:HG3	4	0.18
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	1	0.18
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	1	0.18
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	1	0.18
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	1	0.18
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	7	0.18
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	7	0.18
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	7	0.18
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	7	0.18
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	7	0.18
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	8	0.18
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	3	0.18
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	1	0.18
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	2	0.18
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	4	0.18
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	3	0.18
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	6	0.18
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	9	0.18
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	4	0.18
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	2	0.18
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	2	0.18
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	7	0.18
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	7	0.18
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	4	0.18
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	6	0.18
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	8	0.18
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	6	0.18
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	6	0.18
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	6	0.18
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	9	0.18
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	9	0.18
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	9	0.18
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	5	0.18
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	5	0.18
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	5	0.18
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	9	0.18
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	9	0.18
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	9	0.18
(1,80)	1:7:A:LEU:HB3	1:7:A:LEU:HG	8	0.18
(1,49)	1:6:A:ARG:HE	1:6:A:ARG:HG3	8	0.18
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.18
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	3	0.18
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	4	0.18
(1,18)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.18
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.17
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	9	0.17
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	1	0.17
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	3	0.17
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	5	0.17
(4,28)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	7	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	7	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	7	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	0.17
(4,23)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	0.17
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.17
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.17
(4,20)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.17
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.17
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.17
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	0.17
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	0.17
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	0.17
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.17
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.17
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.17
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.17
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.17
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	0.17
(3,494)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.17
(3,494)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.17
(3,494)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.17
(3,494)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	0.17
(3,494)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	0.17
(3,494)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	0.17
(3,488)	1:10:A:GLN:HA	1:13:A:LYS:HB3	1	0.17
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	0.17
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	0.17
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	0.17
(3,471)	1:8:A:TYR:HA	1:11:A:TRP:H	2	0.17
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	3	0.17
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	3	0.17
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	3	0.17
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	5	0.17
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	5	0.17
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.17
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.17
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	4	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	4	0.17
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	4	0.17
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	5	0.17
(3,367)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	7	0.17
(3,367)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	7	0.17
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.17
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.17
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	9	0.17
(3,235)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.17
(3,33)	1:6:A:ARG:H	1:6:A:ARG:HD2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.17
(2,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	1	0.17
(2,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	1	0.17
(2,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	1	0.17
(2,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	1	0.17
(2,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	1	0.17
(2,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	1	0.17
(2,553)	1:10:A:GLN:HA	1:13:A:LYS:HB3	1	0.17
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	2	0.17
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	2	0.17
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	2	0.17
(2,528)	1:8:A:TYR:HA	1:11:A:TRP:H	2	0.17
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	8	0.17
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	3	0.17
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	3	0.17
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	3	0.17
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	5	0.17
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	5	0.17
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	9	0.17
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	9	0.17
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	9	0.17
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	4	0.17
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	4	0.17
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	4	0.17
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	5	0.17
(2,397)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	7	0.17
(2,397)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	7	0.17
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	9	0.17
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	1	0.17
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	3	0.17
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	5	0.17
(2,346)	1:24:A:PRO:HB3	1:24:A:PRO:HG3	10	0.17
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	2	0.17
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	5	0.17
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	9	0.17
(2,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	6	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	7	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	7	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	7	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	9	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	9	0.17
(2,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG21	6	0.17
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG22	6	0.17
(2,187)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.17
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	6	0.17
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	6	0.17
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	6	0.17
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	9	0.17
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	9	0.17
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	9	0.17
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	10	0.17
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	10	0.17
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	10	0.17
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.17
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.17
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	10	0.17
(2,36)	1:6:A:ARG:H	1:6:A:ARG:HD2	5	0.17
(2,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	4	0.17
(1,557)	1:4:A:ALA:HB1	1:6:A:ARG:HD3	2	0.17
(1,557)	1:4:A:ALA:HB2	1:6:A:ARG:HD3	2	0.17
(1,557)	1:4:A:ALA:HB3	1:6:A:ARG:HD3	2	0.17
(1,522)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	6	0.17
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD21	8	0.17
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD22	8	0.17
(1,464)	1:11:A:TRP:HH2	1:12:A:LEU:HD23	8	0.17
(1,462)	1:6:A:ARG:HG2	1:7:A:LEU:H	4	0.17
(1,454)	1:11:A:TRP:HD1	1:21:A:ARG:HG3	3	0.17
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	6	0.17
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	6	0.17
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	6	0.17
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	6	0.17
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	6	0.17
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	6	0.17
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	6	0.17
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	6	0.17
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	6	0.17
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	6	0.17
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	6	0.17
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	6	0.17
(1,386)	1:10:A:GLN:H	1:11:A:TRP:HB2	10	0.17
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	2	0.17
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	4	0.17
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	6	0.17
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	2	0.17
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	3	0.17
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	3	0.17
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	3	0.17
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	3	0.17
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	8	0.17
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	8	0.17
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	8	0.17
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	8	0.17
(1,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD2	10	0.17
(1,246)	1:13:A:LYS:HB2	1:13:A:LYS:HD3	10	0.17
(1,246)	1:13:A:LYS:HB3	1:13:A:LYS:HD2	10	0.17
(1,246)	1:13:A:LYS:HB3	1:13:A:LYS:HD3	10	0.17
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG2	8	0.17
(1,243)	1:13:A:LYS:HA	1:13:A:LYS:HG3	8	0.17
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	1	0.17
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	7	0.17
(1,211)	1:11:A:TRP:HB3	1:12:A:LEU:H	7	0.17
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	3	0.17
(1,181)	1:9:A:ILE:HG13	1:9:A:ILE:HG21	8	0.17
(1,181)	1:9:A:ILE:HG13	1:9:A:ILE:HG22	8	0.17
(1,181)	1:9:A:ILE:HG13	1:9:A:ILE:HG23	8	0.17
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	5	0.17
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	7	0.17
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	9	0.17
(1,163)	1:8:A:TYR:HB2	1:8:A:TYR:HB3	10	0.17
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	6	0.17
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	10	0.17
(1,122)	1:15:A:GLY:H	1:15:A:GLY:HA2	1	0.17
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	7	0.17
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	9	0.17
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	9	0.17
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD21	8	0.17
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD22	8	0.17
(1,85)	1:7:A:LEU:HB2	1:7:A:LEU:HD23	8	0.17
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	6	0.17
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	6	0.17
(1,66)	1:6:A:ARG:HB2	1:6:A:ARG:HG2	5	0.17
(1,31)	1:5:A:VAL:HA	1:5:A:VAL:HB	10	0.17
(1,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	8	0.17
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	6	0.17
(1,7)	1:3:A:GLU:HB2	1:3:A:GLU:HB3	8	0.17
(4,56)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	4	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	4	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	4	0.16
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	6	0.16
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	10	0.16
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.16
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.16
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.16
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.16
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	0.16
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	0.16
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	0.16
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.16
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.16
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	2	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	2	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	2	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.16
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.16
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	0.16
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.16
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	0.16
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	2	0.16
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	2	0.16
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	4	0.16
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	4	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.16
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	3	0.16
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	3	0.16
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	3	0.16
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	10	0.16
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	10	0.16
(3,367)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	8	0.16
(3,367)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	8	0.16
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	0.16
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	4	0.16
(3,353)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	3	0.16
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	5	0.16
(3,235)	1:14:A:GLN:H	1:14:A:GLN:HG3	1	0.16
(3,93)	1:7:A:LEU:H	1:8:A:TYR:HB2	8	0.16
(2,520)	1:16:A:GLY:H	1:17:A:PRO:HD2	9	0.16
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	4	0.16
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	4	0.16
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	4	0.16
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	2	0.16
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	2	0.16
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	4	0.16
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	4	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	5	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	5	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	5	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	6	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	6	0.16
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	6	0.16
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	3	0.16
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	3	0.16
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	3	0.16
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	10	0.16
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	10	0.16
(2,397)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	8	0.16
(2,397)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	8	0.16
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	4	0.16
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	4	0.16
(2,383)	1:11:A:TRP:HE1	1:21:A:ARG:HG3	3	0.16
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	6	0.16
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	10	0.16
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	5	0.16
(2,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	1	0.16
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	1	0.16
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	10	0.16
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	10	0.16
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	2	0.16
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	2	0.16
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	2	0.16
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	3	0.16
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	3	0.16
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	3	0.16
(2,104)	1:7:A:LEU:H	1:8:A:TYR:HB2	8	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	2	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	2	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	2	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	7	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	7	0.16
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	7	0.16
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	7	0.16
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.16
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	7	0.16
(1,517)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	10	0.16
(1,490)	1:6:A:ARG:HA	1:9:A:ILE:HB	2	0.16
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	8	0.16
(1,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	8	0.16
(1,476)	1:13:A:LYS:HB2	1:14:A:GLN:H	6	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	5	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	5	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	5	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	5	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	5	0.16
(1,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	5	0.16
(1,424)	1:7:A:LEU:HD21	1:24:A:PRO:HB2	9	0.16
(1,424)	1:7:A:LEU:HD22	1:24:A:PRO:HB2	9	0.16
(1,424)	1:7:A:LEU:HD23	1:24:A:PRO:HB2	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG11	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG12	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG13	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG21	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG22	9	0.16
(1,405)	1:4:A:ALA:H	1:5:A:VAL:HG23	9	0.16
(1,380)	1:11:A:TRP:HE1	1:23:A:PRO:HA	1	0.16
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	4	0.16
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:6:A:ARG:HA	1:9:A:ILE:H	5	0.16
(1,297)	1:21:A:ARG:HA	1:21:A:ARG:HB3	9	0.16
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD2	8	0.16
(1,295)	1:21:A:ARG:HA	1:21:A:ARG:HD3	8	0.16
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.16
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	9	0.16
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	9	0.16
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	9	0.16
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	9	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	3	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	5	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	7	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	8	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	9	0.16
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	10	0.16
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	5	0.16
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB2	4	0.16
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB3	4	0.16
(1,179)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.16
(1,179)	1:9:A:ILE:HB	1:9:A:ILE:HD12	4	0.16
(1,179)	1:9:A:ILE:HB	1:9:A:ILE:HD13	4	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	1	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	2	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	3	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	4	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	5	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	7	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	9	0.16
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	10	0.16
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	6	0.16
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	6	0.16
(1,101)	1:8:A:TYR:HA	1:8:A:TYR:HB2	5	0.16
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD11	8	0.16
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD12	8	0.16
(1,94)	1:6:A:ARG:H	1:7:A:LEU:HD13	8	0.16
(1,61)	1:6:A:ARG:HD3	1:6:A:ARG:HG2	5	0.16
(1,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	4	0.16
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB1	4	0.16
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB2	4	0.16
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB3	4	0.16
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	3	0.15
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	3	0.15
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	3	0.15
(4,30)	1:11:A:TRP:HA	1:11:A:TRP:HD1	4	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	1	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	1	0.15
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	1	0.15
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	7	0.15
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	7	0.15
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	7	0.15
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE2	6	0.15
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE3	6	0.15
(3,452)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	10	0.15
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	8	0.15
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	8	0.15
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	8	0.15
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	8	0.15
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	8	0.15
(3,371)	1:24:A:PRO:HG3	1:25:A:SER:H	1	0.15
(3,290)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	0.15
(3,150)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.15
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	2	0.15
(3,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.15
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	7	0.15
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	7	0.15
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	7	0.15
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE2	6	0.15
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE3	6	0.15
(2,501)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	10	0.15
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	3	0.15
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	3	0.15
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	3	0.15
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	8	0.15
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	8	0.15
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	8	0.15
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	8	0.15
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	8	0.15
(2,401)	1:24:A:PRO:HG3	1:25:A:SER:H	1	0.15
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	3	0.15
(2,366)	1:11:A:TRP:HA	1:11:A:TRP:HD1	4	0.15
(2,315)	1:21:A:ARG:H	1:21:A:ARG:HG3	9	0.15
(2,168)	1:8:A:TYR:HB2	1:9:A:ILE:H	3	0.15
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	1	0.15
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	1	0.15
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	2	0.15
(2,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.15
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD2	4	0.15
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD2	4	0.15
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD2	4	0.15
(1,561)	1:9:A:ILE:HG21	1:13:A:LYS:HD3	4	0.15
(1,561)	1:9:A:ILE:HG22	1:13:A:LYS:HD3	4	0.15
(1,561)	1:9:A:ILE:HG23	1:13:A:LYS:HD3	4	0.15
(1,517)	1:16:A:GLY:HA3	1:17:A:PRO:HD2	3	0.15
(1,488)	1:8:A:TYR:HA	1:24:A:PRO:HG3	2	0.15
(1,448)	1:8:A:TYR:HE1	1:23:A:PRO:HB3	8	0.15
(1,448)	1:8:A:TYR:HE2	1:23:A:PRO:HB3	8	0.15
(1,368)	1:11:A:TRP:HH2	1:17:A:PRO:HD3	6	0.15
(1,360)	1:6:A:ARG:HA	1:9:A:ILE:H	3	0.15
(1,319)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	10	0.15
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	1	0.15
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	4	0.15
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	6	0.15
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	6	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	2	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	2	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	2	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	2	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	4	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	4	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	4	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	4	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	6	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	6	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	6	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	6	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG2	10	0.15
(1,248)	1:13:A:LYS:HD2	1:13:A:LYS:HG3	10	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG2	10	0.15
(1,248)	1:13:A:LYS:HD3	1:13:A:LYS:HG3	10	0.15
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	5	0.15
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	5	0.15
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	5	0.15
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	1	0.15
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	1	0.15
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	4	0.15
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	6	0.15
(1,225)	1:12:A:LEU:HA	1:12:A:LEU:HB2	9	0.15
(1,175)	1:9:A:ILE:HA	1:9:A:ILE:HG12	6	0.15
(1,157)	1:14:A:GLN:HE21	1:14:A:GLN:HE22	8	0.15
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	1	0.15
(1,156)	1:10:A:GLN:HE21	1:10:A:GLN:HE22	2	0.15
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	3	0.15
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	5	0.15
(1,109)	1:7:A:LEU:HD21	1:8:A:TYR:H	4	0.15
(1,109)	1:7:A:LEU:HD22	1:8:A:TYR:H	4	0.15
(1,109)	1:7:A:LEU:HD23	1:8:A:TYR:H	4	0.15
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	7	0.15
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	7	0.15
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	7	0.15
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	10	0.15
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	10	0.15
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	10	0.15
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	3	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	4	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	7	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	10	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	10	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	10	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	10	0.15
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	10	0.15
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB1	6	0.15
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB2	6	0.15
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB3	6	0.15
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD11	2	0.14
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD12	2	0.14
(4,49)	1:5:A:VAL:HA	1:7:A:LEU:HD13	2	0.14
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.14
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.14
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.14
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.14
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.14
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	1	0.14
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	1	0.14
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	1	0.14
(3,493)	1:9:A:ILE:HG21	1:12:A:LEU:HG	8	0.14
(3,493)	1:9:A:ILE:HG22	1:12:A:LEU:HG	8	0.14
(3,493)	1:9:A:ILE:HG23	1:12:A:LEU:HG	8	0.14
(3,484)	1:2:A:GLU:HA	1:3:A:GLU:HG2	6	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	5	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	5	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	5	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	9	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	9	0.14
(3,481)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	9	0.14
(3,472)	1:7:A:LEU:HA	1:10:A:GLN:H	7	0.14
(3,470)	1:14:A:GLN:HA	1:16:A:GLY:H	3	0.14
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.14
(3,457)	1:14:A:GLN:HB2	1:16:A:GLY:H	5	0.14
(3,457)	1:14:A:GLN:HB3	1:16:A:GLY:H	5	0.14
(3,457)	1:14:A:GLN:HB2	1:16:A:GLY:H	7	0.14
(3,457)	1:14:A:GLN:HB3	1:16:A:GLY:H	7	0.14
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	6	0.14
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	6	0.14
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	6	0.14
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	2	0.14
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	2	0.14
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	3	0.14
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	3	0.14
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	6	0.14
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	6	0.14
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	6	0.14
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.14
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.14
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.14
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	9	0.14
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	9	0.14
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	9	0.14
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	9	0.14
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	10	0.14
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	10	0.14
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	10	0.14
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	6	0.14
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	6	0.14
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	6	0.14
(3,367)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	5	0.14
(3,367)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	5	0.14
(3,342)	1:17:A:PRO:HD3	1:18:A:SER:H	3	0.14
(3,319)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	3	0.14
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.14
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.14
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.14
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.14
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	1	0.14
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	7	0.14
(2,560)	1:9:A:ILE:HG21	1:12:A:LEU:HG	8	0.14
(2,560)	1:9:A:ILE:HG22	1:12:A:LEU:HG	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:9:A:ILE:HG23	1:12:A:LEU:HG	8	0.14
(2,547)	1:2:A:GLU:HA	1:3:A:GLU:HG2	6	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	5	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	5	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	5	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD11	9	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD12	9	0.14
(2,543)	1:11:A:TRP:HZ3	1:12:A:LEU:HD13	9	0.14
(2,529)	1:7:A:LEU:HA	1:10:A:GLN:H	7	0.14
(2,527)	1:14:A:GLN:HA	1:16:A:GLY:H	3	0.14
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	3	0.14
(2,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	5	0.14
(2,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	5	0.14
(2,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	7	0.14
(2,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	7	0.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD11	2	0.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD12	2	0.14
(2,498)	1:5:A:VAL:HA	1:7:A:LEU:HD13	2	0.14
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	6	0.14
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	6	0.14
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	6	0.14
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	2	0.14
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	2	0.14
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	3	0.14
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	3	0.14
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	6	0.14
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	6	0.14
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	6	0.14
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	6	0.14
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	9	0.14
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	9	0.14
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	9	0.14
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	9	0.14
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	9	0.14
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	9	0.14
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	9	0.14
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	9	0.14
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	9	0.14
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	9	0.14
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	9	0.14
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	10	0.14
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	10	0.14
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	10	0.14
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	6	0.14
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	6	0.14
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	6	0.14
(2,397)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	5	0.14
(2,397)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	5	0.14
(2,372)	1:17:A:PRO:HD3	1:18:A:SER:H	3	0.14
(2,347)	1:24:A:PRO:HB3	1:24:A:PRO:HG2	3	0.14
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	3	0.14
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	6	0.14
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	6	0.14
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	6	0.14
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	3	0.14
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	3	0.14
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	5	0.14
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	5	0.14
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	5	0.14
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	1	0.14
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	1	0.14
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	1	0.14
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	1	0.14
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	7	0.14
(1,552)	1:3:A:GLU:HB2	1:4:A:ALA:HA	2	0.14
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	1	0.14
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	2	0.14
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	8	0.14
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	9	0.14
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG2	4	0.14
(1,503)	1:10:A:GLN:HG3	1:13:A:LYS:HG3	4	0.14
(1,499)	1:5:A:VAL:HG11	1:8:A:TYR:HB2	10	0.14
(1,499)	1:5:A:VAL:HG12	1:8:A:TYR:HB2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:5:A:VAL:HG13	1:8:A:TYR:HB2	10	0.14
(1,499)	1:5:A:VAL:HG21	1:8:A:TYR:HB2	10	0.14
(1,499)	1:5:A:VAL:HG22	1:8:A:TYR:HB2	10	0.14
(1,499)	1:5:A:VAL:HG23	1:8:A:TYR:HB2	10	0.14
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD1	7	0.14
(1,444)	1:7:A:LEU:HD11	1:8:A:TYR:HD2	7	0.14
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD1	7	0.14
(1,444)	1:7:A:LEU:HD12	1:8:A:TYR:HD2	7	0.14
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD1	7	0.14
(1,444)	1:7:A:LEU:HD13	1:8:A:TYR:HD2	7	0.14
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG11	1:7:A:LEU:HD13	10	0.14
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG12	1:7:A:LEU:HD13	10	0.14
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG13	1:7:A:LEU:HD13	10	0.14
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG21	1:7:A:LEU:HD13	10	0.14
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG22	1:7:A:LEU:HD13	10	0.14
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD11	10	0.14
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD12	10	0.14
(1,430)	1:5:A:VAL:HG23	1:7:A:LEU:HD13	10	0.14
(1,402)	1:4:A:ALA:H	1:5:A:VAL:HB	10	0.14
(1,354)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	1	0.14
(1,353)	1:25:A:SER:H	1:25:A:SER:HB2	10	0.14
(1,353)	1:25:A:SER:H	1:25:A:SER:HB3	10	0.14
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	8	0.14
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	1	0.14
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	9	0.14
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	3	0.14
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	3	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	9	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	9	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	9	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	10	0.14
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	10	0.14
(1,228)	1:12:A:LEU:HB2	1:12:A:LEU:HB3	2	0.14
(1,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	3	0.14
(1,167)	1:8:A:TYR:HD1	1:9:A:ILE:H	4	0.14
(1,167)	1:8:A:TYR:HD2	1:9:A:ILE:H	4	0.14
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	6	0.14
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	7	0.14
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	9	0.14
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	6	0.14
(1,83)	1:7:A:LEU:HD21	1:7:A:LEU:HG	8	0.14
(1,83)	1:7:A:LEU:HD22	1:7:A:LEU:HG	8	0.14
(1,83)	1:7:A:LEU:HD23	1:7:A:LEU:HG	8	0.14
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	1	0.14
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	1	0.14
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	1	0.14
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	3	0.14
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	3	0.14
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	3	0.14
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	8	0.14
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	8	0.14
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	8	0.14
(1,46)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.14
(1,41)	1:6:A:ARG:HA	1:6:A:ARG:HB2	5	0.14
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	2	0.14
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	3	0.14
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	4	0.14
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	8	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG21	9	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG22	9	0.14
(1,29)	1:5:A:VAL:H	1:5:A:VAL:HG23	9	0.14
(1,14)	1:3:A:GLU:HA	1:4:A:ALA:H	8	0.14
(1,3)	1:3:A:GLU:HA	1:3:A:GLU:HG2	2	0.14
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.13
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.13
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.13
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.13
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.13
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.13
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.13
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.13
(4,13)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	0.13
(4,13)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	0.13
(4,13)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	0.13
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	5	0.13
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	5	0.13
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	5	0.13
(3,457)	1:14:A:GLN:HB2	1:16:A:GLY:H	9	0.13
(3,457)	1:14:A:GLN:HB3	1:16:A:GLY:H	9	0.13
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE2	4	0.13
(3,453)	1:12:A:LEU:HG	1:13:A:LYS:HE3	4	0.13
(3,448)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.13
(3,448)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.13
(3,448)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.13
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	2	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	2	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	2	0.13
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	5	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	5	0.13
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	5	0.13
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.13
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB3	1	0.13
(3,437)	1:13:A:LYS:H	1:14:A:GLN:HG2	2	0.13
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	1	0.13
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	1	0.13
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	5	0.13
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	5	0.13
(3,407)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	5	0.13
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	5	0.13
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	5	0.13
(3,407)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	5	0.13
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	7	0.13
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	7	0.13
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	7	0.13
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.13
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	4	0.13
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	4	0.13
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	0.13
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	9	0.13
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	1	0.13
(3,275)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,186)	1:10:A:GLN:H	1:10:A:GLN:HE22	9	0.13
(3,82)	1:6:A:ARG:H	1:7:A:LEU:HB2	8	0.13
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	4	0.13
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	8	0.13
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	8	0.13
(2,509)	1:14:A:GLN:HB2	1:16:A:GLY:H	9	0.13
(2,509)	1:14:A:GLN:HB3	1:16:A:GLY:H	9	0.13
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE2	4	0.13
(2,502)	1:12:A:LEU:HG	1:13:A:LYS:HE3	4	0.13
(2,496)	1:6:A:ARG:HA	1:9:A:ILE:HG21	6	0.13
(2,496)	1:6:A:ARG:HA	1:9:A:ILE:HG22	6	0.13
(2,496)	1:6:A:ARG:HA	1:9:A:ILE:HG23	6	0.13
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	2	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	2	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	2	0.13
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	5	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	5	0.13
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	5	0.13
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	1	0.13
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	1	0.13
(2,483)	1:13:A:LYS:H	1:14:A:GLN:HG2	2	0.13
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	1	0.13
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	1	0.13
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD11	5	0.13
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD12	5	0.13
(2,450)	1:8:A:TYR:HE1	1:12:A:LEU:HD13	5	0.13
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD11	5	0.13
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD12	5	0.13
(2,450)	1:8:A:TYR:HE2	1:12:A:LEU:HD13	5	0.13
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	9	0.13
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	9	0.13
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	9	0.13
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	7	0.13
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	7	0.13
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	7	0.13
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	9	0.13
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	4	0.13
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	4	0.13
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	9	0.13
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	9	0.13
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	1	0.13
(2,300)	1:21:A:ARG:HB2	1:21:A:ARG:HD2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	9	0.13
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	2	0.13
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	2	0.13
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	7	0.13
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	7	0.13
(2,108)	1:7:A:LEU:HD11	1:8:A:TYR:H	7	0.13
(2,108)	1:7:A:LEU:HD12	1:8:A:TYR:H	7	0.13
(2,108)	1:7:A:LEU:HD13	1:8:A:TYR:H	7	0.13
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	5	0.13
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	5	0.13
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	5	0.13
(2,92)	1:6:A:ARG:H	1:7:A:LEU:HB2	8	0.13
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	4	0.13
(1,537)	1:6:A:ARG:HB2	1:7:A:LEU:H	3	0.13
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	5	0.13
(1,487)	1:3:A:GLU:HA	1:6:A:ARG:HB3	4	0.13
(1,408)	1:5:A:VAL:HG11	1:9:A:ILE:H	3	0.13
(1,408)	1:5:A:VAL:HG12	1:9:A:ILE:H	3	0.13
(1,408)	1:5:A:VAL:HG13	1:9:A:ILE:H	3	0.13
(1,408)	1:5:A:VAL:HG21	1:9:A:ILE:H	3	0.13
(1,408)	1:5:A:VAL:HG22	1:9:A:ILE:H	3	0.13
(1,408)	1:5:A:VAL:HG23	1:9:A:ILE:H	3	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	2	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	3	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	4	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	5	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	6	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	7	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	8	0.13
(1,323)	1:22:A:PRO:HD2	1:22:A:PRO:HD3	10	0.13
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	5	0.13
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	9	0.13
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	9	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	1	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	1	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	1	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	7	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	7	0.13
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	7	0.13
(1,219)	1:12:A:LEU:HA	1:12:A:LEU:HG	2	0.13
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	6	0.13
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:10:A:GLN:H	1:10:A:GLN:HG2	3	0.13
(1,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	7	0.13
(1,180)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	8	0.13
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	2	0.13
(1,107)	1:7:A:LEU:HB3	1:8:A:TYR:H	8	0.13
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	4	0.13
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	6	0.13
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	2	0.13
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	2	0.13
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	2	0.13
(1,82)	1:7:A:LEU:HD11	1:7:A:LEU:HG	4	0.13
(1,82)	1:7:A:LEU:HD12	1:7:A:LEU:HG	4	0.13
(1,82)	1:7:A:LEU:HD13	1:7:A:LEU:HG	4	0.13
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	1	0.13
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	3	0.13
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	7	0.13
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	10	0.13
(1,60)	1:6:A:ARG:HB3	1:6:A:ARG:HD3	3	0.13
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	6	0.13
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	5	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	9	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	9	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	9	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	9	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	9	0.13
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	9	0.13
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB1	9	0.13
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB2	9	0.13
(1,15)	1:4:A:ALA:H	1:4:A:ALA:HB3	9	0.13
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.12
(4,60)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.12
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.12
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.12
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.12
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	6	0.12
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	6	0.12
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.12
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.12
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.12
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD11	3	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD12	3	0.12
(4,8)	1:7:A:LEU:H	1:7:A:LEU:HD13	3	0.12
(3,471)	1:8:A:TYR:HA	1:11:A:TRP:H	8	0.12
(3,456)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.12
(3,456)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.12
(3,452)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	3	0.12
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	4	0.12
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	4	0.12
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	4	0.12
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	7	0.12
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	7	0.12
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	7	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.12
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.12
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	9	0.12
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	9	0.12
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	9	0.12
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.12
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	3	0.12
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	3	0.12
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	0.12
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	5	0.12
(3,289)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,186)	1:10:A:GLN:H	1:10:A:GLN:HE22	2	0.12
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	1	0.12
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	3	0.12
(3,34)	1:6:A:ARG:H	1:6:A:ARG:HD3	10	0.12
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB2	7	0.12
(2,536)	1:7:A:LEU:H	1:10:A:GLN:HB3	7	0.12
(2,528)	1:8:A:TYR:HA	1:11:A:TRP:H	8	0.12
(2,507)	1:10:A:GLN:HB2	1:11:A:TRP:H	3	0.12
(2,507)	1:10:A:GLN:HB3	1:11:A:TRP:H	3	0.12
(2,501)	1:23:A:PRO:HB2	1:24:A:PRO:HD2	3	0.12
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	4	0.12
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	4	0.12
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	4	0.12
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	7	0.12
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	7	0.12
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	7	0.12
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	5	0.12
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	5	0.12
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	5	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	1	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	1	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	1	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	2	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	2	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	2	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	7	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	7	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	7	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	10	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	10	0.12
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	10	0.12
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	9	0.12
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	9	0.12
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	9	0.12
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	7	0.12
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	3	0.12
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	3	0.12
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	5	0.12
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	5	0.12
(2,314)	1:21:A:ARG:H	1:21:A:ARG:HB3	10	0.12
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	6	0.12
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	6	0.12
(2,206)	1:10:A:GLN:H	1:10:A:GLN:HE22	2	0.12
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	1	0.12
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	5	0.12
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	5	0.12
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	9	0.12
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	9	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	2	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	2	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	2	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD11	3	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD12	3	0.12
(2,87)	1:7:A:LEU:H	1:7:A:LEU:HD13	3	0.12
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	3	0.12
(2,37)	1:6:A:ARG:H	1:6:A:ARG:HD3	10	0.12
(1,538)	1:10:A:GLN:HE21	1:14:A:GLN:HG2	10	0.12
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	7	0.12
(1,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB1	8	0.12
(1,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB2	8	0.12
(1,427)	1:3:A:GLU:HB3	1:4:A:ALA:HB3	8	0.12
(1,395)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	5	0.12
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	7	0.12
(1,341)	1:24:A:PRO:HD3	1:24:A:PRO:HG2	9	0.12
(1,319)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	2	0.12
(1,319)	1:22:A:PRO:HB3	1:22:A:PRO:HD3	4	0.12
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	2	0.12
(1,298)	1:21:A:ARG:HA	1:21:A:ARG:HG2	7	0.12
(1,292)	1:19:A:SER:H	1:20:A:GLY:H	8	0.12
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	2	0.12
(1,272)	1:15:A:GLY:HA2	1:16:A:GLY:H	3	0.12
(1,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	4	0.12
(1,260)	1:14:A:GLN:H	1:14:A:GLN:HG3	9	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	5	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	5	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	8	0.12
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	8	0.12
(1,253)	1:15:A:GLY:H	1:16:A:GLY:H	7	0.12
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE2	1	0.12
(1,239)	1:13:A:LYS:H	1:13:A:LYS:HE3	1	0.12
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	2	0.12
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	7	0.12
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:10:A:GLN:HA	1:10:A:GLN:HB3	10	0.12
(1,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	4	0.12
(1,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	4	0.12
(1,182)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	4	0.12
(1,180)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	1	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	4	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	4	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	4	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	6	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	6	0.12
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	6	0.12
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	8	0.12
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	10	0.12
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	10	0.12
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	2	0.12
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	4	0.12
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	9	0.12
(1,71)	1:5:A:VAL:H	1:7:A:LEU:H	1	0.12
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	8	0.12
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	10	0.12
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	1	0.12
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	7	0.12
(1,39)	1:6:A:ARG:HD2	1:6:A:ARG:HE	10	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	1	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	2	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	2	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	2	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	2	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	2	0.12
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	2	0.12
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB1	3	0.12
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB2	3	0.12
(1,25)	1:3:A:GLU:H	1:4:A:ALA:HB3	3	0.12
(1,2)	1:2:A:GLU:HA	1:3:A:GLU:H	6	0.12
(4,41)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	5	0.11
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD11	4	0.11
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:12:A:LEU:H	1:12:A:LEU:HD13	4	0.11
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.11
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.11
(4,11)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.11
(3,495)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.11
(3,495)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.11
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	1	0.11
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	0.11
(3,480)	1:17:A:PRO:HG2	1:18:A:SER:H	3	0.11
(3,480)	1:17:A:PRO:HG3	1:18:A:SER:H	3	0.11
(3,476)	1:16:A:GLY:H	1:19:A:SER:HB3	6	0.11
(3,472)	1:7:A:LEU:HA	1:10:A:GLN:H	2	0.11
(3,472)	1:7:A:LEU:HA	1:10:A:GLN:H	4	0.11
(3,460)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.11
(3,440)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.11
(3,429)	1:11:A:TRP:HE1	1:19:A:SER:HG	1	0.11
(3,425)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.11
(3,417)	1:12:A:LEU:HB2	1:13:A:LYS:H	8	0.11
(3,413)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	5	0.11
(3,413)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	5	0.11
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	7	0.11
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	7	0.11
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	9	0.11
(3,411)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	9	0.11
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.11
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.11
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.11
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	10	0.11
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	10	0.11
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	10	0.11
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	10	0.11
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.11
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.11
(3,392)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.11
(3,381)	1:9:A:ILE:HG21	1:11:A:TRP:H	8	0.11
(3,381)	1:9:A:ILE:HG22	1:11:A:TRP:H	8	0.11
(3,381)	1:9:A:ILE:HG23	1:11:A:TRP:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD11	5	0.11
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD12	5	0.11
(3,376)	1:3:A:GLU:H	1:7:A:LEU:HD13	5	0.11
(3,370)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.11
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	5	0.11
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	5	0.11
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	9	0.11
(3,368)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	9	0.11
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	0.11
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	7	0.11
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	0.11
(3,363)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	8	0.11
(3,359)	1:11:A:TRP:HZ3	1:12:A:LEU:HA	7	0.11
(3,342)	1:17:A:PRO:HD3	1:18:A:SER:H	7	0.11
(3,340)	1:9:A:ILE:HA	1:10:A:GLN:HE22	4	0.11
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD1	3	0.11
(3,339)	1:5:A:VAL:HA	1:8:A:TYR:HD2	3	0.11
(3,326)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	4	0.11
(3,256)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	4	0.11
(3,256)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	4	0.11
(3,241)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD11	5	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD12	5	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD13	5	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD11	9	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD12	9	0.11
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD13	9	0.11
(3,166)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.11
(2,563)	1:8:A:TYR:HE1	1:11:A:TRP:HE3	10	0.11
(2,563)	1:8:A:TYR:HE2	1:11:A:TRP:HE3	10	0.11
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	1	0.11
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	7	0.11
(2,542)	1:17:A:PRO:HG2	1:18:A:SER:H	3	0.11
(2,542)	1:17:A:PRO:HG3	1:18:A:SER:H	3	0.11
(2,534)	1:16:A:GLY:H	1:19:A:SER:HB3	6	0.11
(2,529)	1:7:A:LEU:HA	1:10:A:GLN:H	2	0.11
(2,529)	1:7:A:LEU:HA	1:10:A:GLN:H	4	0.11
(2,513)	1:11:A:TRP:HD1	1:24:A:PRO:HD2	8	0.11
(2,487)	1:3:A:GLU:HA	1:6:A:ARG:HB3	8	0.11
(2,474)	1:11:A:TRP:HE1	1:19:A:SER:HG	1	0.11
(2,469)	1:11:A:TRP:HH2	1:17:A:PRO:HD2	4	0.11
(2,461)	1:12:A:LEU:HB2	1:13:A:LYS:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,457)	1:8:A:TYR:HD1	1:24:A:PRO:HB3	5	0.11
(2,457)	1:8:A:TYR:HD2	1:24:A:PRO:HB3	5	0.11
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	7	0.11
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	7	0.11
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG2	9	0.11
(2,455)	1:11:A:TRP:HD1	1:22:A:PRO:HG3	9	0.11
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	10	0.11
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	10	0.11
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	10	0.11
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	10	0.11
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	10	0.11
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	10	0.11
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	10	0.11
(2,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	5	0.11
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD21	3	0.11
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD22	3	0.11
(2,428)	1:7:A:LEU:HB3	1:7:A:LEU:HD23	3	0.11
(2,413)	1:9:A:ILE:HG21	1:11:A:TRP:H	8	0.11
(2,413)	1:9:A:ILE:HG22	1:11:A:TRP:H	8	0.11
(2,413)	1:9:A:ILE:HG23	1:11:A:TRP:H	8	0.11
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD11	5	0.11
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD12	5	0.11
(2,407)	1:3:A:GLU:H	1:7:A:LEU:HD13	5	0.11
(2,400)	1:24:A:PRO:HB3	1:25:A:SER:H	4	0.11
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	5	0.11
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	5	0.11
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG2	9	0.11
(2,398)	1:11:A:TRP:HE3	1:17:A:PRO:HG3	9	0.11
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	7	0.11
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	7	0.11
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG2	8	0.11
(2,393)	1:11:A:TRP:HZ2	1:17:A:PRO:HG3	8	0.11
(2,389)	1:11:A:TRP:HZ3	1:12:A:LEU:HA	7	0.11
(2,372)	1:17:A:PRO:HD3	1:18:A:SER:H	7	0.11
(2,370)	1:9:A:ILE:HA	1:10:A:GLN:HE22	4	0.11
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD1	3	0.11
(2,369)	1:5:A:VAL:HA	1:8:A:TYR:HD2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,354)	1:11:A:TRP:HZ2	1:17:A:PRO:HA	4	0.11
(2,281)	1:17:A:PRO:HB3	1:17:A:PRO:HG2	4	0.11
(2,281)	1:17:A:PRO:HB3	1:17:A:PRO:HG3	4	0.11
(2,266)	1:14:A:GLN:HA	1:14:A:GLN:HG2	3	0.11
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD11	4	0.11
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD12	4	0.11
(2,221)	1:12:A:LEU:H	1:12:A:LEU:HD13	4	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	5	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	5	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	5	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	9	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	9	0.11
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	9	0.11
(2,185)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.11
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD21	10	0.11
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD22	10	0.11
(2,93)	1:6:A:ARG:H	1:7:A:LEU:HD23	10	0.11
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	3	0.11
(1,441)	1:6:A:ARG:HD2	1:6:A:ARG:HH11	9	0.11
(1,374)	1:5:A:VAL:HA	1:7:A:LEU:H	5	0.11
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	5	0.11
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	10	0.11
(1,316)	1:21:A:ARG:H	1:21:A:ARG:HB2	5	0.11
(1,258)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	9	0.11
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB2	7	0.11
(1,255)	1:14:A:GLN:HA	1:14:A:GLN:HB3	7	0.11
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	3	0.11
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD21	4	0.11
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD22	4	0.11
(1,220)	1:12:A:LEU:H	1:12:A:LEU:HD23	4	0.11
(1,207)	1:11:A:TRP:H	1:12:A:LEU:H	5	0.11
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	2	0.11
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	9	0.11
(1,194)	1:10:A:GLN:HB2	1:10:A:GLN:HE21	2	0.11
(1,194)	1:10:A:GLN:HB3	1:10:A:GLN:HE21	2	0.11
(1,180)	1:9:A:ILE:HG12	1:9:A:ILE:HG13	2	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	1	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	1	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	1	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	2	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	2	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	3	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	3	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	3	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	7	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	7	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	7	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	8	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	8	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	8	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	10	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	10	0.11
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	10	0.11
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD1	1	0.11
(1,113)	1:8:A:TYR:HB2	1:8:A:TYR:HD2	1	0.11
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	2	0.11
(1,100)	1:8:A:TYR:H	1:8:A:TYR:HB3	9	0.11
(1,96)	1:7:A:LEU:H	1:8:A:TYR:H	8	0.11
(1,91)	1:6:A:ARG:H	1:7:A:LEU:HB3	3	0.11
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	5	0.11
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	6	0.11
(1,53)	1:5:A:VAL:H	1:6:A:ARG:HB2	3	0.11
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	1	0.11
(1,42)	1:6:A:ARG:HA	1:6:A:ARG:HB3	2	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	6	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG11	8	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG12	8	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG13	8	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG21	8	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG22	8	0.11
(1,33)	1:5:A:VAL:HB	1:5:A:VAL:HG23	8	0.11
(1,28)	1:4:A:ALA:HA	1:5:A:VAL:H	5	0.11
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.1
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.1
(4,40)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.1
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.1
(4,14)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.1
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,485)	1:2:A:GLU:HA	1:5:A:VAL:HB	8	0.1
(3,476)	1:16:A:GLY:H	1:19:A:SER:HB3	2	0.1
(3,445)	1:17:A:PRO:HG2	1:18:A:SER:HB2	9	0.1
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB2	9	0.1
(3,445)	1:17:A:PRO:HG3	1:18:A:SER:HB3	9	0.1
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.1
(3,442)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.1
(3,436)	1:10:A:GLN:HB2	1:13:A:LYS:H	9	0.1
(3,436)	1:10:A:GLN:HB3	1:13:A:LYS:H	9	0.1
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.1
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.1
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.1
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	7	0.1
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	7	0.1
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	7	0.1
(3,408)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	7	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG11	4	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG12	4	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG13	4	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG21	4	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG22	4	0.1
(3,396)	1:2:A:GLU:HA	1:5:A:VAL:HG23	4	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG21	7	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG22	7	0.1
(3,395)	1:4:A:ALA:HA	1:5:A:VAL:HG23	7	0.1
(3,382)	1:12:A:LEU:HD21	1:16:A:GLY:H	5	0.1
(3,382)	1:12:A:LEU:HD22	1:16:A:GLY:H	5	0.1
(3,382)	1:12:A:LEU:HD23	1:16:A:GLY:H	5	0.1
(3,367)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	9	0.1
(3,367)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	9	0.1
(3,349)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	4	0.1
(3,232)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	6	0.1
(3,208)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.1
(3,208)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,208)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.1
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD11	7	0.1
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD12	7	0.1
(3,194)	1:12:A:LEU:HA	1:12:A:LEU:HD13	7	0.1
(3,172)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.1
(3,138)	1:24:A:PRO:HA	1:24:A:PRO:HD3	2	0.1
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.1
(3,97)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.1
(3,16)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.1
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	6	0.1
(2,548)	1:2:A:GLU:HA	1:5:A:VAL:HB	8	0.1
(2,534)	1:16:A:GLY:H	1:19:A:SER:HB3	2	0.1
(2,492)	1:17:A:PRO:HG2	1:18:A:SER:HB2	9	0.1
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB2	9	0.1
(2,492)	1:17:A:PRO:HG3	1:18:A:SER:HB3	9	0.1
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB2	2	0.1
(2,489)	1:7:A:LEU:HA	1:10:A:GLN:HB3	2	0.1
(2,482)	1:10:A:GLN:HB2	1:13:A:LYS:H	9	0.1
(2,482)	1:10:A:GLN:HB3	1:13:A:LYS:H	9	0.1
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG11	1:8:A:TYR:HE2	7	0.1
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG12	1:8:A:TYR:HE2	7	0.1
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG13	1:8:A:TYR:HE2	7	0.1
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG21	1:8:A:TYR:HE2	7	0.1
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG22	1:8:A:TYR:HE2	7	0.1
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE1	7	0.1
(2,451)	1:5:A:VAL:HG23	1:8:A:TYR:HE2	7	0.1
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD21	7	0.1
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD22	7	0.1
(2,440)	1:11:A:TRP:HE3	1:12:A:LEU:HD23	7	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG11	4	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG12	4	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG13	4	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG21	4	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG22	4	0.1
(2,433)	1:2:A:GLU:HA	1:5:A:VAL:HG23	4	0.1
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG11	7	0.1
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG12	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG13	7	0.1
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG21	7	0.1
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG22	7	0.1
(2,432)	1:4:A:ALA:HA	1:5:A:VAL:HG23	7	0.1
(2,414)	1:12:A:LEU:HD21	1:16:A:GLY:H	5	0.1
(2,414)	1:12:A:LEU:HD22	1:16:A:GLY:H	5	0.1
(2,414)	1:12:A:LEU:HD23	1:16:A:GLY:H	5	0.1
(2,397)	1:10:A:GLN:HB2	1:10:A:GLN:HE22	9	0.1
(2,397)	1:10:A:GLN:HB3	1:10:A:GLN:HE22	9	0.1
(2,379)	1:11:A:TRP:HB3	1:11:A:TRP:HE1	4	0.1
(2,257)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	6	0.1
(2,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD21	2	0.1
(2,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD22	2	0.1
(2,232)	1:12:A:LEU:HB2	1:12:A:LEU:HD23	2	0.1
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD11	7	0.1
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD12	7	0.1
(2,215)	1:12:A:LEU:HA	1:12:A:LEU:HD13	7	0.1
(2,192)	1:10:A:GLN:HA	1:10:A:GLN:HG3	2	0.1
(2,155)	1:24:A:PRO:HA	1:24:A:PRO:HD3	2	0.1
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE1	4	0.1
(2,111)	1:8:A:TYR:HB2	1:8:A:TYR:HE2	4	0.1
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE1	8	0.1
(2,110)	1:8:A:TYR:HB3	1:8:A:TYR:HE2	8	0.1
(2,19)	1:3:A:GLU:H	1:3:A:GLU:HG3	2	0.1
(1,519)	1:16:A:GLY:H	1:17:A:PRO:HD3	10	0.1
(1,442)	1:6:A:ARG:HD3	1:6:A:ARG:HH11	2	0.1
(1,410)	1:5:A:VAL:HG11	1:8:A:TYR:H	1	0.1
(1,410)	1:5:A:VAL:HG12	1:8:A:TYR:H	1	0.1
(1,410)	1:5:A:VAL:HG13	1:8:A:TYR:H	1	0.1
(1,410)	1:5:A:VAL:HG21	1:8:A:TYR:H	1	0.1
(1,410)	1:5:A:VAL:HG22	1:8:A:TYR:H	1	0.1
(1,410)	1:5:A:VAL:HG23	1:8:A:TYR:H	1	0.1
(1,401)	1:24:A:PRO:HG3	1:25:A:SER:H	2	0.1
(1,395)	1:10:A:GLN:HE22	1:10:A:GLN:HG2	9	0.1
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	1	0.1
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	3	0.1
(1,343)	1:24:A:PRO:HB2	1:24:A:PRO:HB3	9	0.1
(1,252)	1:13:A:LYS:H	1:14:A:GLN:H	9	0.1
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD11	3	0.1
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD12	3	0.1
(1,233)	1:12:A:LEU:HB2	1:12:A:LEU:HD13	3	0.1
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:11:A:TRP:HA	1:11:A:TRP:HB2	8	0.1
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB2	7	0.1
(1,193)	1:10:A:GLN:H	1:10:A:GLN:HB3	7	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	5	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	5	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	5	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG21	9	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG22	9	0.1
(1,172)	1:9:A:ILE:HB	1:9:A:ILE:HG23	9	0.1
(1,126)	1:18:A:SER:H	1:18:A:SER:HA	10	0.1
(1,91)	1:6:A:ARG:H	1:7:A:LEU:HB3	2	0.1
(1,91)	1:6:A:ARG:H	1:7:A:LEU:HB3	4	0.1
(1,79)	1:7:A:LEU:HB2	1:7:A:LEU:HB3	8	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found