



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6XTT / pdb_00006xtt
BMRB ID : 34480
Title : Solution structure of Legionella pneumophila NttA
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Deposited on : 2020-01-16

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

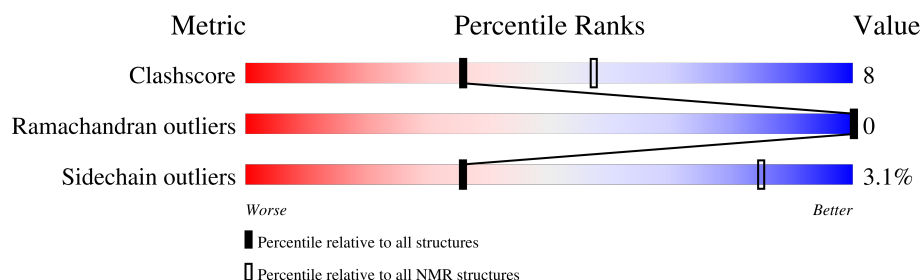
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	B	116	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:8-B:99 (92)	0.41	2

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1827 atoms, of which 898 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NttA.

Mol	Chain	Residues	Atoms						Trace
1	B	116	Total	C	H	N	O	S	0
			1827	579	898	157	183	10	

There are 15 discrepancies between the modelled and reference sequences:

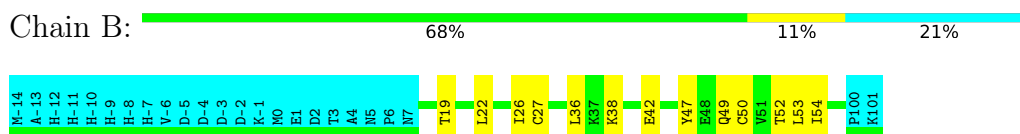
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	MET	-	initiating methionine	UNP A0A128USX4
B	-13	ALA	-	expression tag	UNP A0A128USX4
B	-12	HIS	-	expression tag	UNP A0A128USX4
B	-11	HIS	-	expression tag	UNP A0A128USX4
B	-10	HIS	-	expression tag	UNP A0A128USX4
B	-9	HIS	-	expression tag	UNP A0A128USX4
B	-8	HIS	-	expression tag	UNP A0A128USX4
B	-7	HIS	-	expression tag	UNP A0A128USX4
B	-6	VAL	-	expression tag	UNP A0A128USX4
B	-5	ASP	-	expression tag	UNP A0A128USX4
B	-4	ASP	-	expression tag	UNP A0A128USX4
B	-3	ASP	-	expression tag	UNP A0A128USX4
B	-2	ASP	-	expression tag	UNP A0A128USX4
B	-1	LYS	-	expression tag	UNP A0A128USX4
B	0	MET	-	expression tag	UNP A0A128USX4

4 Residue-property plots [i](#)

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: NttA

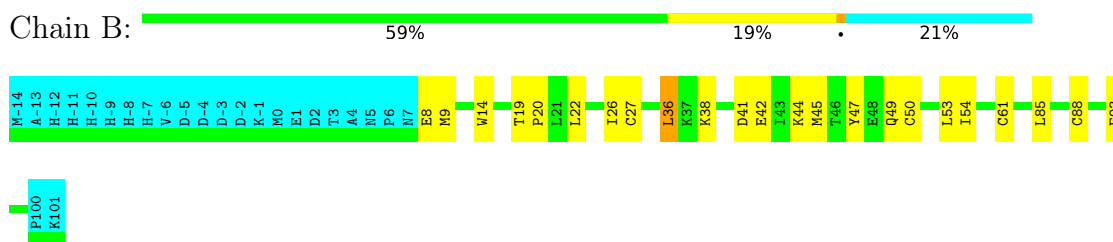


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

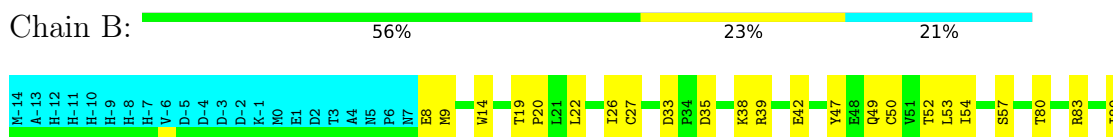
4.2.1 Score per residue for model 1

- Molecule 1: NttA



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: NttA





4.2.3 Score per residue for model 3

- Molecule 1: NttA

Chain B: 64% 15% 21%



4.2.4 Score per residue for model 4

- Molecule 1: NttA

Chain B: 62% 16% 21%



4.2.5 Score per residue for model 5

- Molecule 1: NttA

Chain B: 66% 13% 21%



4.2.6 Score per residue for model 6

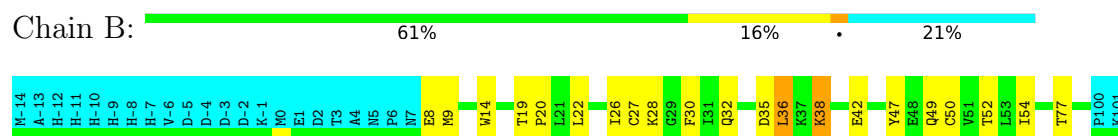
- Molecule 1: NttA

Chain B: 66% 11% 21%



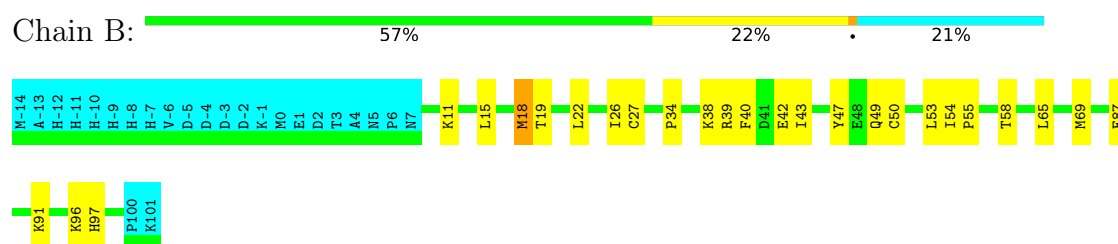
4.2.7 Score per residue for model 7

- Molecule 1: NttA



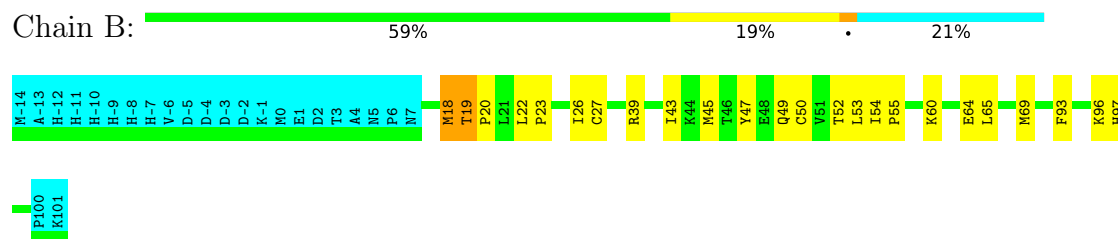
4.2.8 Score per residue for model 8

- Molecule 1: NttA



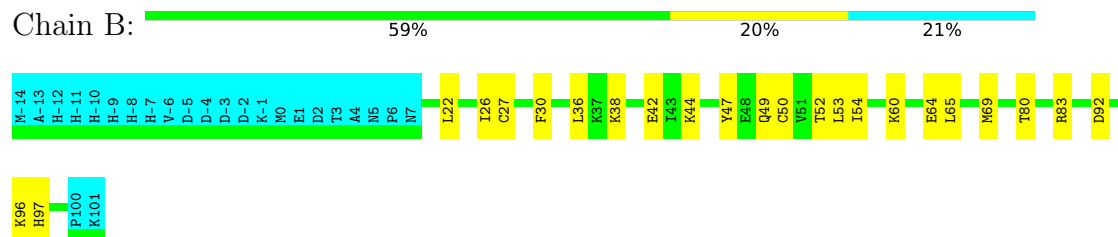
4.2.9 Score per residue for model 9

- Molecule 1: NttA



4.2.10 Score per residue for model 10

- Molecule 1: NttA



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1342
Number of shifts mapped to atoms	1342
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	731	726	727	11±3
All	All	7310	7260	7262	113

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:CYS:SG	1:B:47:TYR:HA	0.78	2.18	4	8
1:B:15:LEU:HA	1:B:18:MET:SD	0.74	2.22	8	1
1:B:49:GLN:O	1:B:53:LEU:HG	0.59	1.97	1	7
1:B:35:ASP:O	1:B:38:LYS:HG3	0.59	1.98	7	2
1:B:38:LYS:O	1:B:42:GLU:HG2	0.58	1.98	8	9
1:B:22:LEU:O	1:B:26:ILE:HG12	0.55	2.02	7	10
1:B:49:GLN:O	1:B:52:THR:HG22	0.55	2.01	2	6
1:B:50:CYS:O	1:B:54:ILE:HG12	0.55	2.01	8	8
1:B:41:ASP:O	1:B:44:LYS:HD2	0.52	2.04	1	1
1:B:61:CYS:SG	1:B:85:LEU:HA	0.52	2.45	1	1
1:B:45:MET:SD	1:B:93:PHE:HZ	0.51	2.28	9	2
1:B:61:CYS:SG	1:B:88:CYS:CB	0.51	2.99	1	1
1:B:55:PRO:HA	1:B:58:THR:OG1	0.51	2.06	8	2
1:B:36:LEU:CD2	1:B:36:LEU:N	0.50	2.74	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:57:SER:OG	1:B:89:ILE:HA	0.49	2.07	2	1
1:B:80:THR:O	1:B:83:ARG:HG2	0.48	2.08	2	2
1:B:9:MET:SD	1:B:14:TRP:HD1	0.47	2.33	7	4
1:B:60:LYS:O	1:B:64:GLU:HG2	0.46	2.11	9	2
1:B:87:GLU:O	1:B:91:LYS:HG3	0.46	2.10	8	1
1:B:92:ASP:OD1	1:B:96:LYS:HE2	0.46	2.10	2	2
1:B:40:PHE:HE1	1:B:50:CYS:SG	0.46	2.34	8	1
1:B:39:ARG:HD2	1:B:98:LEU:O	0.45	2.10	2	1
1:B:53:LEU:HD13	1:B:97:HIS:CD2	0.45	2.46	2	1
1:B:30:PHE:CD1	1:B:36:LEU:HD12	0.45	2.47	6	2
1:B:65:LEU:O	1:B:69:MET:HG3	0.45	2.12	9	5
1:B:11:LYS:O	1:B:15:LEU:HG	0.44	2.12	8	1
1:B:19:THR:OG1	1:B:20:PRO:HD3	0.43	2.14	4	5
1:B:11:LYS:HE2	1:B:66:TYR:CE2	0.43	2.48	4	1
1:B:96:LYS:CG	1:B:97:HIS:N	0.42	2.81	8	2
1:B:18:MET:HA	1:B:18:MET:HE3	0.42	1.90	9	1
1:B:39:ARG:O	1:B:43:ILE:HG12	0.42	2.13	8	3
1:B:91:LYS:O	1:B:95:GLU:HG3	0.42	2.15	4	1
1:B:30:PHE:CD2	1:B:36:LEU:HD13	0.42	2.50	10	1
1:B:45:MET:SD	1:B:93:PHE:CZ	0.41	3.13	1	2
1:B:54:ILE:N	1:B:55:PRO:CD	0.41	2.83	8	5
1:B:34:PRO:O	1:B:38:LYS:HG3	0.41	2.15	8	1
1:B:33:ASP:OD2	1:B:35:ASP:HB2	0.41	2.14	2	1
1:B:28:LYS:O	1:B:32:GLN:HG3	0.40	2.16	7	1
1:B:79:GLY:O	1:B:83:ARG:HG2	0.40	2.16	4	1
1:B:22:LEU:N	1:B:23:PRO:CD	0.40	2.84	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	B	92/116 (79%)	91±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	920/1160 (79%)	907 (99%)	13 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	83/105 (79%)	80±1 (97±1%)	3±1 (3±1%)	36	85
All	All	830/1050 (79%)	804 (97%)	26 (3%)	36	85

All 11 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	36	LEU	6
1	B	19	THR	5
1	B	8	GLU	4
1	B	77	THR	2
1	B	38	LYS	2
1	B	18	MET	2
1	B	64	GLU	1
1	B	63	ASP	1
1	B	62	GLN	1
1	B	44	LYS	1
1	B	97	HIS	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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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	1342
Number of shifts mapped to atoms	1342
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	109	-0.51 ± 0.18	Should be checked
$^{13}\text{C}_\beta$	104	0.04 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	-0.32 ± 0.18	None needed (< 0.5 ppm)
^{15}N	101	0.60 ± 0.19	Should be applied

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 93%, i.e. 1164 atoms were assigned a chemical shift out of a possible 1245. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	452/455 (99%)	184/184 (100%)	181/184 (98%)	87/87 (100%)
Sidechain	646/710 (91%)	439/459 (96%)	207/230 (90%)	0/21 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	66/80 (82%)	34/39 (87%)	30/37 (81%)	2/4 (50%)
Overall	1164/1245 (93%)	657/682 (96%)	418/451 (93%)	89/112 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1342 atoms were assigned a chemical shift out of a possible 1556. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	531/571 (93%)	215/230 (93%)	215/232 (93%)	101/109 (93%)
Sidechain	745/857 (87%)	505/552 (91%)	240/280 (86%)	0/25 (0%)
Aromatic	66/128 (52%)	34/63 (54%)	30/49 (61%)	2/16 (12%)
Overall	1342/1556 (86%)	754/845 (89%)	485/561 (86%)	103/150 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

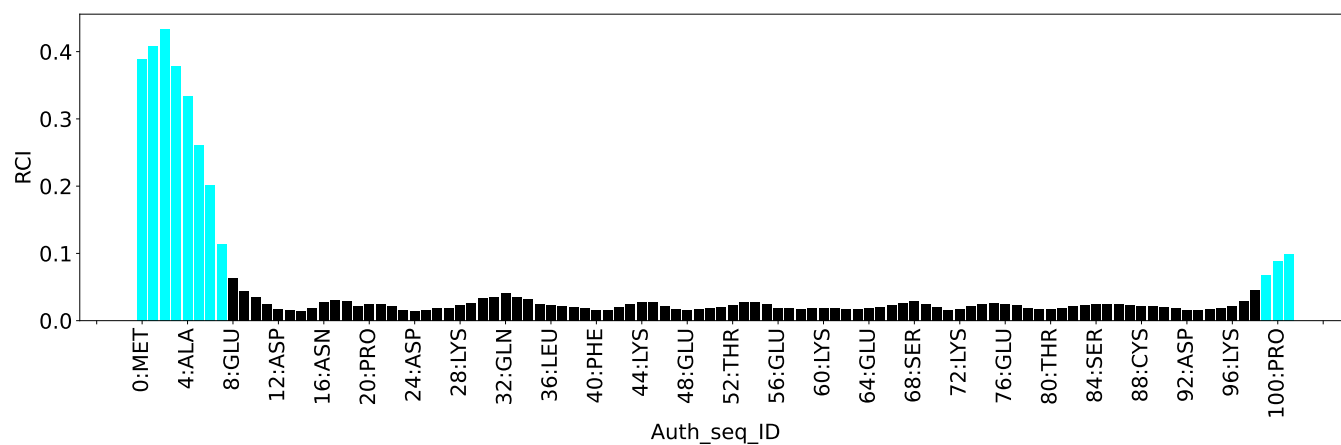
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	18	MET	CE	33.56	8.39 – 25.85	9.4
1	B	0	MET	CE	32.28	8.39 – 25.85	8.7

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain B:



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	3063
Intra-residue ($ i-j =0$)	953
Sequential ($ i-j =1$)	696
Medium range ($ i-j >1$ and $ i-j <5$)	784
Long range ($ i-j \geq 5$)	630
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	26.4
Number of long range restraints per residue ¹	5.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	109.5	0.2
0.2-0.5 (Medium)	238.8	0.5
>0.5 (Large)	252.7	3.21

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 ⓘ

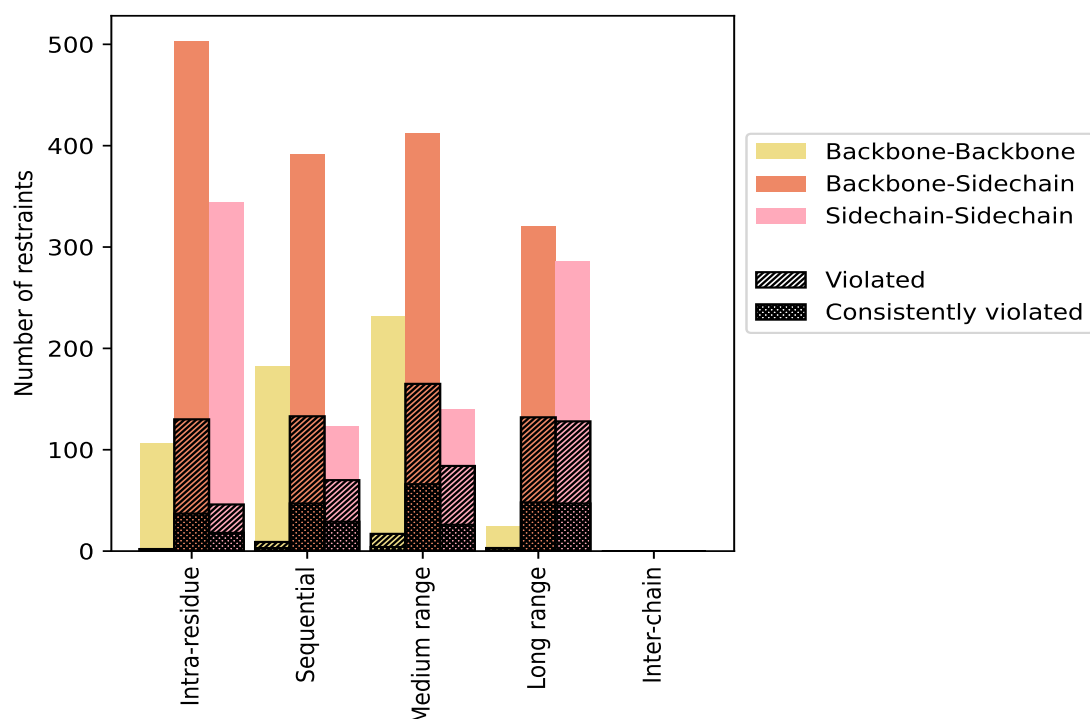
9.1 Summary of distance violations ⓘ

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)	953	31.1	178	18.7	5.8	57	6.0	1.9
Backbone-Backbone	106	3.5	2	1.9	0.1	2	1.9	0.1
Backbone-Sidechain	503	16.4	130	25.8	4.2	37	7.4	1.2
Sidechain-Sidechain	344	11.2	46	13.4	1.5	18	5.2	0.6
Sequential (i-j =1)	696	22.7	212	30.5	6.9	79	11.4	2.6
Backbone-Backbone	182	5.9	9	4.9	0.3	3	1.6	0.1
Backbone-Sidechain	391	12.8	133	34.0	4.3	47	12.0	1.5
Sidechain-Sidechain	123	4.0	70	56.9	2.3	29	23.6	0.9
Medium range (i-j >1 & i-j <5)	784	25.6	266	33.9	8.7	96	12.2	3.1
Backbone-Backbone	232	7.6	17	7.3	0.6	4	1.7	0.1
Backbone-Sidechain	412	13.5	165	40.0	5.4	66	16.0	2.2
Sidechain-Sidechain	140	4.6	84	60.0	2.7	26	18.6	0.8
Long range (i-j ≥5)	630	20.6	263	41.7	8.6	98	15.6	3.2
Backbone-Backbone	24	0.8	3	12.5	0.1	3	12.5	0.1
Backbone-Sidechain	320	10.4	132	41.2	4.3	48	15.0	1.6
Sidechain-Sidechain	286	9.3	128	44.8	4.2	47	16.4	1.5
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	3063	100.0	919	30.0	30.0	330	10.8	10.8
Backbone-Backbone	544	17.8	31	5.7	1.0	12	2.2	0.4
Backbone-Sidechain	1626	53.1	560	34.4	18.3	198	12.2	6.5
Sidechain-Sidechain	893	29.2	328	36.7	10.7	120	13.4	3.9

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

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



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

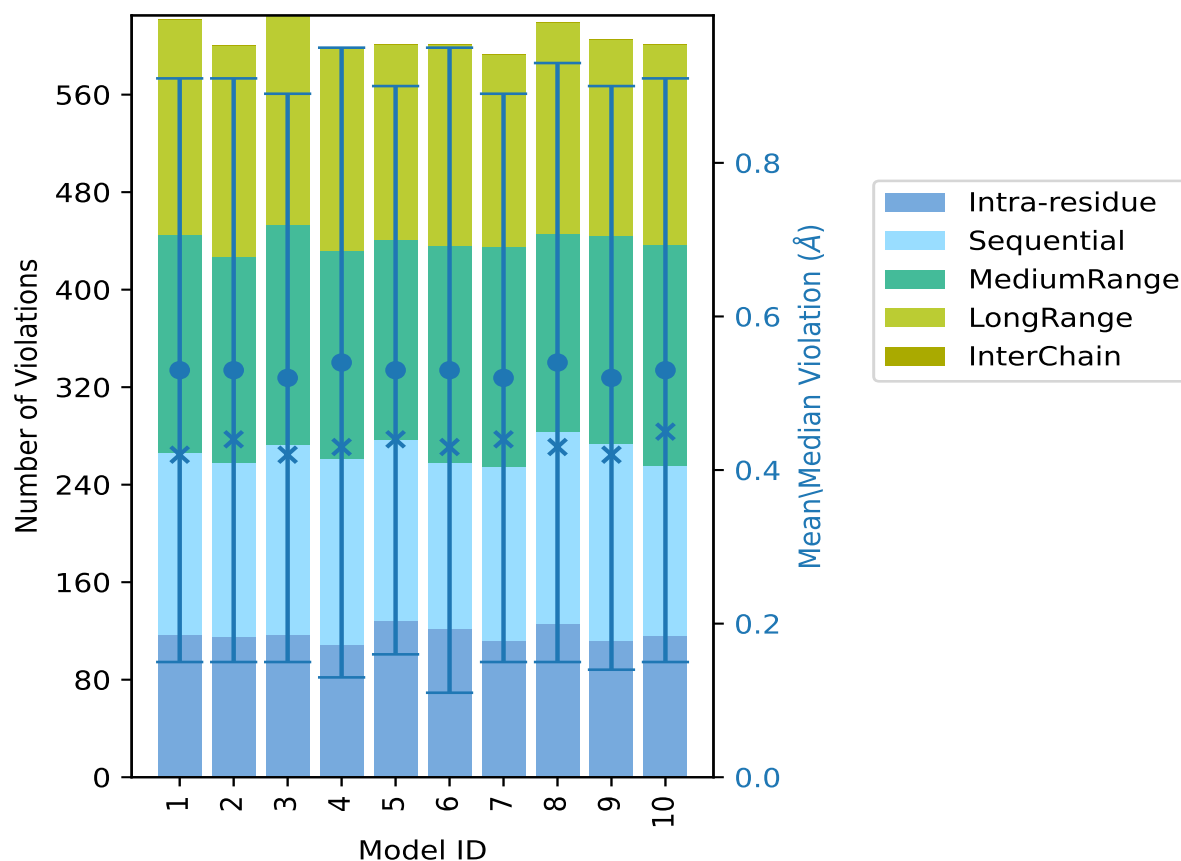
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	117	149	179	177	0	622	0.53	2.67	0.38	0.42
2	115	143	169	173	0	600	0.53	2.78	0.38	0.44
3	117	156	180	172	0	625	0.52	2.7	0.37	0.42
4	109	152	171	166	0	598	0.54	2.91	0.41	0.43
5	128	149	164	160	0	601	0.53	2.42	0.37	0.44
6	122	136	178	165	0	601	0.53	3.21	0.42	0.43
7	112	143	180	158	0	593	0.52	2.51	0.37	0.44
8	126	157	163	173	0	619	0.54	2.66	0.39	0.43
9	112	162	170	161	0	605	0.52	2.77	0.38	0.42
10	116	139	182	164	0	601	0.53	2.72	0.38	0.45

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 [i](#)



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 [i](#)

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, 2144(IR:775, SQ:484, MR:518, LR:367, 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	%
33	35	23	32	0	123	1	10.0
9	20	15	16	0	60	2	20.0
15	11	14	17	0	57	3	30.0

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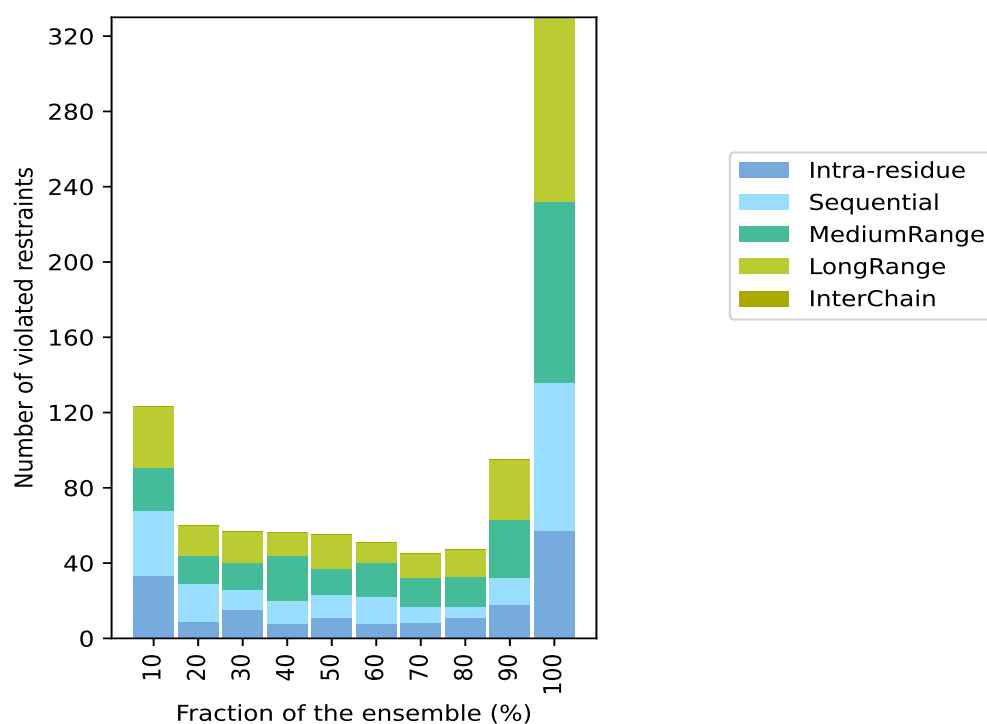
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
8	12	24	12	0	56	4	40.0
11	12	14	18	0	55	5	50.0
8	14	18	11	0	51	6	60.0
8	9	15	13	0	45	7	70.0
11	6	16	14	0	47	8	80.0
18	14	31	32	0	95	9	90.0
57	79	96	98	0	330	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 ⓘ

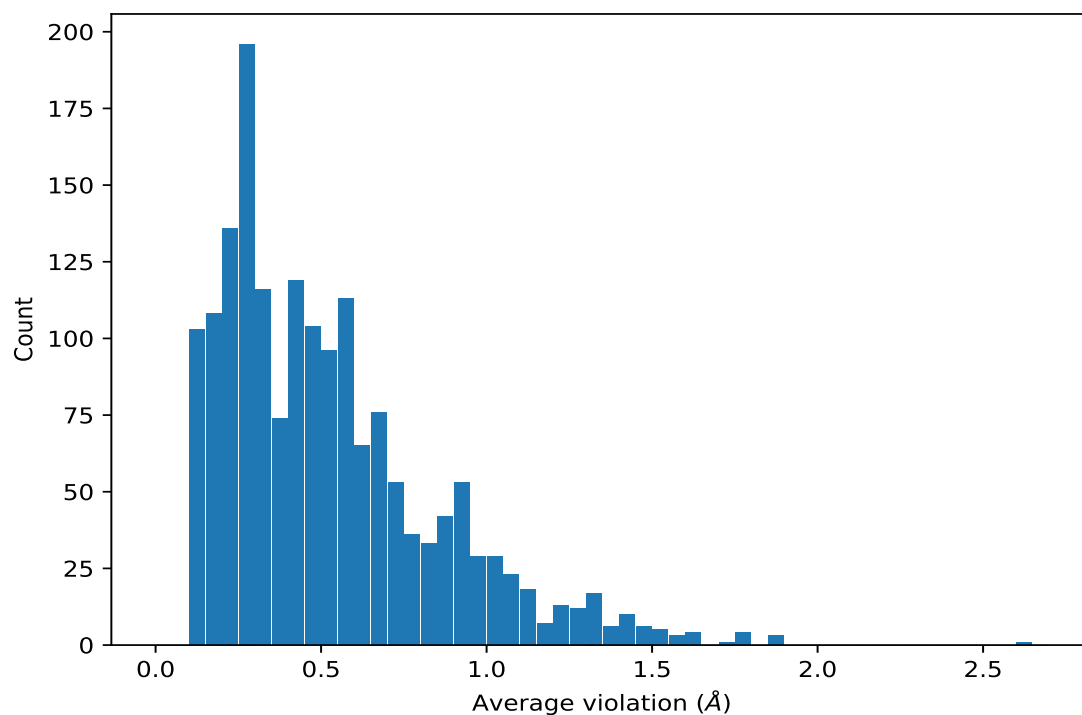


9.4 Most violated distance restraints in the ensemble ⓘ

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)
(2,682)	1:80:B:THR:HG23	1:83:B:ARG:HB3	10	1.88	0.27	1.79
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	10	1.88	0.27	1.79
(2,682)	1:80:B:THR:HG21	1:83:B:ARG:HB3	10	1.88	0.27	1.79
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	10	1.75	0.08	1.76
(2,1004)	1:58:B:THR:HG23	1:20:B:PRO:HB2	10	1.75	0.1	1.79
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	10	1.75	0.1	1.79
(2,1004)	1:58:B:THR:HG22	1:20:B:PRO:HB2	10	1.75	0.1	1.79
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	10	1.71	0.1	1.7
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	10	1.64	0.04	1.65
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	10	1.59	0.13	1.63
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	10	1.5	0.08	1.52
(2,256)	1:52:B:THR:HB	1:49:B:GLN:HG3	10	1.5	0.08	1.52
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG21	10	1.5	0.06	1.5
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	10	1.5	0.06	1.5
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG22	10	1.5	0.06	1.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG23	10	1.47	0.1	1.44
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG22	10	1.47	0.1	1.44
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG21	10	1.47	0.1	1.44
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD13	10	1.46	0.29	1.55
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD11	10	1.46	0.29	1.55
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD12	10	1.46	0.29	1.55
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	10	1.45	0.43	1.5
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD23	10	1.45	0.43	1.5
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD22	10	1.45	0.43	1.5
(2,1122)	1:51:B:VAL:HG13	1:23:B:PRO:HD3	10	1.4	0.03	1.4
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	10	1.4	0.03	1.4
(2,1122)	1:51:B:VAL:HG11	1:23:B:PRO:HD3	10	1.4	0.03	1.4
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	10	1.37	0.18	1.42
(2,974)	1:95:B:GLU:HG3	1:99:B:ILE:HB	10	1.37	0.18	1.42
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	10	1.33	0.65	1.75
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	10	1.32	0.23	1.23
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD11	10	1.32	0.23	1.23
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB1	10	1.32	0.06	1.32
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	10	1.32	0.06	1.32
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB2	10	1.32	0.06	1.32
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD13	10	1.31	0.59	1.22
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	10	1.31	0.59	1.22
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD11	10	1.31	0.59	1.22
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD12	10	1.31	0.59	1.22
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	10	1.31	0.12	1.32
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD13	10	1.3	0.24	1.34
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG23	10	1.3	0.24	1.34
(2,127)	1:50:B:CYS:HB2	1:45:B:MET:HE3	10	1.3	0.24	1.34
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG21	10	1.3	0.24	1.34
(2,127)	1:50:B:CYS:HB2	1:45:B:MET:HE2	10	1.3	0.24	1.34
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD11	10	1.3	0.24	1.34
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	10	1.27	0.34	1.19
(2,564)	1:85:B:LEU:HD12	1:82:B:GLY:HA3	10	1.27	0.34	1.19
(2,564)	1:36:B:LEU:HD21	1:30:B:PHE:HA	10	1.27	0.34	1.19
(2,564)	1:85:B:LEU:HD13	1:82:B:GLY:HA3	10	1.27	0.34	1.19
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD11	10	1.27	0.07	1.27
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD12	10	1.27	0.07	1.27
(2,667)	1:98:B:LEU:HD13	1:39:B:ARG:H	10	1.27	0.07	1.27
(2,667)	1:98:B:LEU:HD11	1:39:B:ARG:H	10	1.27	0.07	1.27
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD13	10	1.27	0.07	1.27
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	10	1.26	0.03	1.28
(2,824)	1:73:B:ILE:HG23	1:70:B:PRO:HG3	10	1.24	0.04	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,824)	1:73:B:ILE:HG21	1:70:B:PRO:HG3	10	1.24	0.04	1.25
(2,824)	1:73:B:ILE:HG22	1:70:B:PRO:HG3	10	1.24	0.04	1.25
(2,236)	1:9:B:MET:HG3	1:72:B:LYS:HB3	10	1.24	0.32	1.3
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	10	1.24	0.32	1.3
(2,236)	1:9:B:MET:HG3	1:18:B:MET:HB2	10	1.24	0.32	1.3
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG22	10	1.24	0.03	1.23
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG21	10	1.24	0.03	1.23
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG23	10	1.24	0.03	1.23
(2,1164)	1:54:B:ILE:HD13	1:55:B:PRO:HD2	10	1.22	0.06	1.2
(2,1164)	1:54:B:ILE:HD12	1:55:B:PRO:HD2	10	1.22	0.06	1.2
(2,1164)	1:54:B:ILE:HD11	1:55:B:PRO:HD2	10	1.22	0.06	1.2
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	10	1.21	0.09	1.23
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	10	1.19	0.14	1.16
(2,1106)	1:10:B:THR:HG23	1:71:B:ASP:HA	10	1.19	0.13	1.15
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	10	1.19	0.13	1.15
(2,1106)	1:10:B:THR:HG21	1:71:B:ASP:HA	10	1.19	0.13	1.15
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	10	1.16	0.07	1.15
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	10	1.16	0.17	1.19
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	10	1.14	0.1	1.16
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG22	10	1.12	0.33	1.22
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	10	1.12	0.33	1.22
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG23	10	1.12	0.33	1.22
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD2	10	1.11	0.53	1.12
(2,943)	1:71:B:ASP:HB2	1:72:B:LYS:HB2	10	1.11	0.53	1.12
(2,943)	1:13:B:ALA:HB2	1:12:B:ASP:HB2	10	1.11	0.53	1.12
(2,943)	1:35:B:ASP:HB3	1:38:B:LYS:HG2	10	1.11	0.53	1.12
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD3	10	1.11	0.53	1.12
(2,827)	1:73:B:ILE:HG21	1:74:B:ASN:HB2	10	1.09	0.21	1.13
(2,827)	1:73:B:ILE:HG22	1:74:B:ASN:HB2	10	1.09	0.21	1.13
(2,827)	1:73:B:ILE:HG23	1:74:B:ASN:HB2	10	1.09	0.21	1.13
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	10	1.08	0.68	0.92
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD23	10	1.08	0.68	0.92
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD22	10	1.08	0.68	0.92
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB3	10	1.08	0.04	1.08
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	10	1.08	0.04	1.08
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB1	10	1.08	0.04	1.08
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB2	10	1.08	0.04	1.08
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	10	1.07	0.71	0.84
(1,798)	1:85:B:LEU:HD21	1:64:B:GLU:H	10	1.07	0.71	0.84
(1,798)	1:85:B:LEU:HD23	1:64:B:GLU:H	10	1.07	0.71	0.84
(2,825)	1:73:B:ILE:HG21	1:9:B:MET:HE3	10	1.06	0.3	1.08
(2,825)	1:73:B:ILE:HG22	1:18:B:MET:HG2	10	1.06	0.3	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,825)	1:73:B:ILE:HG22	1:9:B:MET:HE2	10	1.06	0.3	1.08
(2,825)	1:73:B:ILE:HG21	1:18:B:MET:HG2	10	1.06	0.3	1.08
(2,825)	1:73:B:ILE:HG22	1:9:B:MET:HE3	10	1.06	0.3	1.08
(2,825)	1:73:B:ILE:HG23	1:9:B:MET:HE1	10	1.06	0.3	1.08
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	10	1.06	0.06	1.04
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	10	1.04	0.09	1.04
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG22	10	1.03	0.2	1.01
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG23	10	1.03	0.2	1.01
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG21	10	1.03	0.2	1.01
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	10	1.02	0.04	1.02
(2,490)	1:81:B:TRP:HE3	1:85:B:LEU:HG	10	1.02	0.04	1.02
(2,1168)	1:54:B:ILE:HD11	1:58:B:THR:HG21	10	1.02	0.08	1.02
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG22	10	1.02	0.08	1.02
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG21	10	1.02	0.08	1.02
(2,1168)	1:54:B:ILE:HD12	1:58:B:THR:HG22	10	1.02	0.08	1.02
(2,1168)	1:54:B:ILE:HD12	1:58:B:THR:HG23	10	1.02	0.08	1.02
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	10	1.02	0.26	1.08
(2,1369)	1:58:B:THR:H	1:60:B:LYS:HD3	10	1.02	0.26	1.08
(2,1369)	1:58:B:THR:H	1:59:B:LYS:HD3	10	1.02	0.26	1.08
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	10	1.02	0.27	1.08
(2,286)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	10	1.02	0.27	1.08
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB3	10	1.0	0.06	0.98
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	1.0	0.06	0.98
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB2	10	1.0	0.06	0.98
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	10	0.98	0.22	1.02
(2,627)	1:15:B:LEU:HD11	1:14:B:TRP:H	10	0.98	0.22	1.02
(2,627)	1:65:B:LEU:HD21	1:85:B:LEU:H	10	0.98	0.22	1.02
(2,627)	1:65:B:LEU:HD22	1:85:B:LEU:H	10	0.98	0.22	1.02
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD22	10	0.98	0.17	1.01
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD21	10	0.98	0.17	1.01
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD23	10	0.98	0.17	1.01
(2,638)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	10	0.98	0.17	1.01
(2,272)	1:85:B:LEU:HB3	1:19:B:THR:HA	10	0.98	0.09	0.98
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	10	0.98	0.09	0.98
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	10	0.98	0.11	0.98
(1,569)	1:89:B:ILE:HG21	1:90:B:GLY:HA3	10	0.98	0.11	0.98
(1,569)	1:89:B:ILE:HG22	1:90:B:GLY:HA3	10	0.98	0.11	0.98
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD11	10	0.97	0.07	0.98
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD12	10	0.97	0.07	0.98
(2,1100)	1:98:B:LEU:HD13	1:39:B:ARG:H	10	0.97	0.07	0.98
(2,1100)	1:98:B:LEU:HD11	1:39:B:ARG:H	10	0.97	0.07	0.98
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD13	10	0.97	0.07	0.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	10	0.97	0.21	0.9
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	10	0.97	0.15	0.98
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	10	0.95	0.24	0.86
(2,140)	1:64:B:GLU:HG3	1:60:B:LYS:HG3	10	0.94	0.15	1.01
(2,140)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	10	0.94	0.15	1.01
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	10	0.94	0.15	1.01
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	10	0.94	0.15	1.01
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB3	10	0.94	0.15	1.01
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	10	0.94	0.08	0.94
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB2	10	0.94	0.08	0.94
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG21	10	0.94	0.17	0.99
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG22	10	0.94	0.17	0.99
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG23	10	0.94	0.17	0.99
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG23	10	0.94	0.17	0.99
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG21	10	0.94	0.17	0.99
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG22	10	0.94	0.17	0.99
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	10	0.93	0.31	0.84
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	10	0.93	0.31	0.84
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE1	10	0.92	0.55	0.67
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE3	10	0.92	0.55	0.67
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE2	10	0.92	0.55	0.67
(2,885)	1:90:B:GLY:HA3	1:36:B:LEU:HD12	10	0.92	0.55	0.67
(2,885)	1:90:B:GLY:HA3	1:36:B:LEU:HD13	10	0.92	0.55	0.67
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	10	0.92	0.28	0.98
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	10	0.91	0.26	0.98
(2,554)	1:89:B:ILE:H	1:85:B:LEU:HD13	10	0.91	0.26	0.98
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	10	0.91	0.13	0.94
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	10	0.9	0.06	0.92
(2,84)	1:12:B:ASP:HB3	1:10:B:THR:HG22	10	0.9	0.06	0.92
(2,84)	1:12:B:ASP:HB3	1:10:B:THR:HG21	10	0.9	0.06	0.92
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD13	10	0.9	0.06	0.9
(2,872)	1:26:B:ILE:HD11	1:25:B:LEU:H	10	0.9	0.06	0.9
(2,872)	1:26:B:ILE:HD13	1:25:B:LEU:H	10	0.9	0.06	0.9
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD11	10	0.9	0.06	0.9
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG23	10	0.9	0.04	0.88
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG21	10	0.9	0.04	0.88
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	10	0.9	0.04	0.88
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	10	0.9	0.6	0.88
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	10	0.89	0.07	0.87
(2,211)	1:38:B:LYS:HB3	1:37:B:LYS:H	10	0.89	0.07	0.87
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	10	0.88	0.06	0.86
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD12	10	0.88	0.06	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD13	10	0.88	0.06	0.86
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	10	0.88	0.07	0.89
(2,1273)	1:62:B:GLN:H	1:60:B:LYS:HB2	10	0.88	0.07	0.89
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD12	10	0.87	0.13	0.86
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD13	10	0.87	0.13	0.86
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD11	10	0.87	0.13	0.86
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	10	0.87	0.24	0.9
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	10	0.86	0.08	0.88
(2,592)	1:44:B:LYS:HG3	1:42:B:GLU:HA	10	0.86	0.08	0.88
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	10	0.86	0.12	0.8
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG21	10	0.86	0.17	0.91
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG22	10	0.86	0.17	0.91
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG23	10	0.86	0.17	0.91
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG23	10	0.86	0.17	0.91
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG21	10	0.86	0.17	0.91
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG22	10	0.86	0.17	0.91
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	10	0.86	0.09	0.86
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB2	10	0.86	0.07	0.88
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB3	10	0.86	0.07	0.88
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	10	0.86	0.07	0.88
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD3	10	0.86	0.37	0.96
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	10	0.86	0.37	0.96
(2,144)	1:56:B:GLU:HG3	1:53:B:LEU:HG	10	0.86	0.37	0.96
(2,144)	1:95:B:GLU:HG3	1:99:B:ILE:HB	10	0.86	0.37	0.96
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	10	0.85	0.03	0.84
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	10	0.84	0.16	0.8
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB3	10	0.84	0.16	0.8
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	10	0.84	0.18	0.88
(2,628)	1:65:B:LEU:HD21	1:68:B:SER:HB2	10	0.84	0.18	0.88
(2,628)	1:65:B:LEU:HD23	1:68:B:SER:HB3	10	0.84	0.18	0.88
(2,628)	1:65:B:LEU:HD23	1:68:B:SER:HB2	10	0.84	0.18	0.88
(2,662)	1:77:B:THR:HG23	1:70:B:PRO:HB3	10	0.84	0.06	0.86
(2,662)	1:77:B:THR:HG22	1:70:B:PRO:HB3	10	0.84	0.06	0.86
(2,662)	1:77:B:THR:HG21	1:70:B:PRO:HB3	10	0.84	0.06	0.86
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD23	10	0.83	0.43	0.74
(2,1103)	1:36:B:LEU:HD11	1:35:B:ASP:HB2	10	0.83	0.43	0.74
(2,1103)	1:36:B:LEU:HD12	1:35:B:ASP:HB2	10	0.83	0.43	0.74
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD21	10	0.83	0.43	0.74
(2,1103)	1:36:B:LEU:HD13	1:35:B:ASP:HB2	10	0.83	0.43	0.74
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD22	10	0.83	0.43	0.74
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	10	0.83	0.02	0.83
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	10	0.81	0.13	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	10	0.81	0.09	0.84
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	10	0.8	0.02	0.8
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	10	0.8	0.1	0.8
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	10	0.8	0.13	0.8
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	10	0.79	0.05	0.8
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG21	10	0.79	0.05	0.8
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG22	10	0.79	0.05	0.8
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	10	0.78	0.16	0.68
(2,1116)	1:19:B:THR:HG23	1:62:B:GLN:HA	10	0.78	0.16	0.68
(2,1116)	1:19:B:THR:HG21	1:62:B:GLN:HA	10	0.78	0.16	0.68
(2,1051)	1:51:B:VAL:HG22	1:48:B:GLU:HB2	10	0.78	0.08	0.79
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	10	0.78	0.08	0.79
(2,1051)	1:51:B:VAL:HG23	1:48:B:GLU:HB2	10	0.78	0.08	0.79
(2,1165)	1:54:B:ILE:HD12	1:50:B:CYS:HB2	10	0.78	0.27	0.89
(2,1165)	1:54:B:ILE:HD11	1:50:B:CYS:HB2	10	0.78	0.27	0.89
(2,1165)	1:54:B:ILE:HD13	1:50:B:CYS:HB2	10	0.78	0.27	0.89
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	10	0.77	0.13	0.82
(2,1107)	1:88:B:CYS:HA	1:89:B:ILE:HB	10	0.77	0.13	0.82
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	10	0.76	0.27	0.67
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	10	0.75	0.06	0.74
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG23	10	0.75	0.06	0.74
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG21	10	0.75	0.06	0.74
(2,1120)	1:67:B:ALA:HB3	1:68:B:SER:HA	10	0.75	0.06	0.76
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	10	0.75	0.06	0.76
(2,1120)	1:99:B:ILE:HA	1:98:B:LEU:HB2	10	0.75	0.06	0.76
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	10	0.75	0.17	0.8
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	10	0.75	0.02	0.74
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	10	0.75	0.11	0.78
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	10	0.75	0.11	0.78
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	10	0.75	0.14	0.73
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	10	0.74	0.33	0.76
(2,1030)	1:54:B:ILE:HG12	1:27:B:CYS:HB3	10	0.74	0.33	0.76
(2,1030)	1:44:B:LYS:HD3	1:41:B:ASP:HB2	10	0.74	0.33	0.76
(2,774)	1:78:B:ALA:HB2	1:80:B:THR:H	10	0.74	0.09	0.75
(2,774)	1:78:B:ALA:HB3	1:80:B:THR:H	10	0.74	0.09	0.75
(2,774)	1:78:B:ALA:HB1	1:80:B:THR:H	10	0.74	0.09	0.75
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	10	0.74	0.35	0.62
(2,1017)	1:64:B:GLU:HG2	1:60:B:LYS:HD2	10	0.74	0.35	0.62
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD2	10	0.74	0.35	0.62
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	10	0.73	0.15	0.68
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD22	10	0.72	0.16	0.68
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG21	10	0.72	0.16	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD21	10	0.72	0.16	0.68
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG22	10	0.72	0.16	0.68
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG23	10	0.72	0.16	0.68
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD11	10	0.72	0.05	0.73
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD13	10	0.72	0.05	0.73
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	10	0.72	0.05	0.73
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	10	0.72	0.08	0.72
(2,322)	1:41:B:ASP:H	1:39:B:ARG:HB3	10	0.72	0.08	0.72
(2,773)	1:67:B:ALA:HB3	1:68:B:SER:HA	10	0.72	0.07	0.71
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	10	0.72	0.07	0.71
(2,773)	1:67:B:ALA:HB1	1:68:B:SER:HA	10	0.72	0.07	0.71
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD23	10	0.72	0.22	0.72
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD11	10	0.72	0.22	0.72
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD22	10	0.72	0.22	0.72
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD12	10	0.72	0.22	0.72
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD13	10	0.72	0.22	0.72
(2,1043)	1:48:B:GLU:HB3	1:52:B:THR:H	10	0.72	0.21	0.73
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	10	0.72	0.21	0.73
(2,1043)	1:33:B:ASP:H	1:37:B:LYS:HD3	10	0.72	0.21	0.73
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	10	0.72	0.05	0.72
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD13	10	0.72	0.05	0.72
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD22	10	0.71	0.73	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD23	10	0.71	0.73	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD21	10	0.71	0.73	0.47
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD12	10	0.7	0.12	0.68
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD11	10	0.7	0.12	0.68
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD13	10	0.7	0.12	0.68
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG23	10	0.7	0.12	0.72
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	10	0.7	0.12	0.72
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG21	10	0.7	0.12	0.72
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	10	0.69	0.09	0.72
(2,921)	1:84:B:SER:HB2	1:81:B:TRP:HZ3	10	0.69	0.09	0.72
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	10	0.69	0.15	0.66
(2,643)	1:45:B:MET:HB2	1:40:B:PHE:HA	10	0.68	0.28	0.7
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	10	0.68	0.28	0.7
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	10	0.68	0.06	0.7
(2,1023)	1:89:B:ILE:HG13	1:61:B:CYS:HA	10	0.68	0.06	0.7
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	10	0.68	0.1	0.72
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB3	10	0.68	0.1	0.72
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE2	10	0.68	0.1	0.72
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB1	10	0.68	0.1	0.72
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB2	10	0.68	0.1	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD13	10	0.68	0.23	0.66
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD11	10	0.68	0.23	0.66
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE2	10	0.68	0.23	0.66
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE1	10	0.68	0.23	0.66
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE3	10	0.68	0.23	0.66
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG23	10	0.68	0.1	0.7
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG22	10	0.68	0.1	0.7
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG21	10	0.68	0.1	0.7
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	10	0.67	0.14	0.67
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	10	0.67	0.1	0.68
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	10	0.67	0.1	0.71
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HB	10	0.67	0.1	0.71
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	10	0.67	0.15	0.7
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD13	10	0.67	0.15	0.7
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD11	10	0.67	0.15	0.7
(2,108)	1:30:B:PHE:HB2	1:36:B:LEU:HD11	10	0.67	0.15	0.7
(2,664)	1:57:B:SER:H	1:58:B:THR:HG21	10	0.66	0.08	0.62
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	10	0.66	0.08	0.62
(2,664)	1:57:B:SER:H	1:58:B:THR:HG23	10	0.66	0.08	0.62
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	10	0.66	0.15	0.63
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD13	10	0.65	0.09	0.69
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD12	10	0.65	0.09	0.69
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD11	10	0.65	0.09	0.69
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG21	10	0.65	0.09	0.68
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	10	0.65	0.09	0.68
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG22	10	0.65	0.09	0.68
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	10	0.65	0.12	0.62
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.65	0.03	0.65
(2,200)	1:69:B:MET:HB2	1:11:B:LYS:HA	10	0.64	0.1	0.68
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	10	0.64	0.1	0.68
(2,200)	1:18:B:MET:HB2	1:82:B:GLY:HA2	10	0.64	0.1	0.68
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	10	0.64	0.03	0.64
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	10	0.63	0.03	0.64
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD23	10	0.63	0.07	0.62
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	10	0.63	0.07	0.62
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD21	10	0.63	0.07	0.62
(1,485)	1:98:B:LEU:HD22	1:40:B:PHE:HB3	10	0.63	0.29	0.59
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	10	0.63	0.29	0.59
(1,485)	1:98:B:LEU:HD23	1:40:B:PHE:HB3	10	0.63	0.29	0.59
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD21	10	0.63	0.25	0.59
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD21	10	0.63	0.25	0.59
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD23	10	0.63	0.25	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD22	10	0.63	0.25	0.59
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD22	10	0.63	0.25	0.59
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	10	0.63	0.15	0.66
(2,975)	1:54:B:ILE:HB	1:50:B:CYS:HA	10	0.63	0.15	0.66
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	10	0.63	0.15	0.64
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB3	10	0.63	0.15	0.64
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	10	0.62	0.14	0.6
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD21	10	0.62	0.21	0.62
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD22	10	0.62	0.21	0.62
(2,928)	1:65:B:LEU:HB3	1:85:B:LEU:HD12	10	0.62	0.21	0.62
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD23	10	0.62	0.21	0.62
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	10	0.62	0.08	0.64
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	10	0.62	0.13	0.59
(2,896)	1:73:B:ILE:HD11	1:69:B:MET:HA	10	0.62	0.13	0.59
(2,896)	1:69:B:MET:HE2	1:69:B:MET:HA	10	0.62	0.13	0.59
(2,896)	1:73:B:ILE:HD12	1:69:B:MET:HA	10	0.62	0.13	0.59
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	10	0.61	0.04	0.61
(2,495)	1:81:B:TRP:HE3	1:85:B:LEU:HG	10	0.61	0.04	0.61
(1,574)	1:78:B:ALA:HB2	1:77:B:THR:H	10	0.61	0.02	0.6
(1,574)	1:78:B:ALA:HB3	1:77:B:THR:H	10	0.61	0.02	0.6
(1,574)	1:78:B:ALA:HB1	1:77:B:THR:H	10	0.61	0.02	0.6
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD1	10	0.6	0.19	0.55
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD1	10	0.6	0.19	0.55
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD2	10	0.6	0.19	0.55
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD2	10	0.6	0.19	0.55
(1,827)	1:89:B:ILE:HG21	1:93:B:PHE:HD1	10	0.6	0.19	0.55
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG22	10	0.6	0.12	0.56
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG23	10	0.6	0.12	0.56
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	10	0.6	0.12	0.56
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	10	0.6	0.14	0.67
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	10	0.6	0.14	0.67
(1,841)	1:54:B:ILE:HD11	1:23:B:PRO:HB3	10	0.59	0.15	0.58
(1,841)	1:54:B:ILE:HD13	1:23:B:PRO:HB3	10	0.59	0.15	0.58
(1,841)	1:54:B:ILE:HD12	1:23:B:PRO:HB3	10	0.59	0.15	0.58
(2,154)	1:56:B:GLU:HG3	1:53:B:LEU:HB3	10	0.59	0.21	0.59
(2,154)	1:56:B:GLU:HG3	1:96:B:LYS:HD2	10	0.59	0.21	0.59
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	10	0.59	0.21	0.59
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD11	10	0.59	0.12	0.64
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD13	10	0.59	0.12	0.64
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD12	10	0.59	0.12	0.64
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	10	0.59	0.02	0.58
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG22	10	0.59	0.19	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG23	10	0.59	0.19	0.59
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG21	10	0.59	0.19	0.59
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG23	10	0.58	0.06	0.6
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	10	0.58	0.06	0.6
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG21	10	0.58	0.06	0.6
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	10	0.58	0.07	0.56
(2,1009)	1:66:B:TYR:HA	1:11:B:LYS:HB3	10	0.58	0.07	0.56
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	10	0.57	0.04	0.57
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	10	0.57	0.04	0.57
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	10	0.57	0.04	0.57
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	10	0.57	0.02	0.58
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG23	10	0.57	0.02	0.58
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG22	10	0.57	0.02	0.58
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	10	0.57	0.04	0.58
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	10	0.57	0.22	0.57
(2,822)	1:73:B:ILE:HG21	1:75:B:SER:HA	10	0.56	0.15	0.57
(2,822)	1:73:B:ILE:HG22	1:11:B:LYS:HA	10	0.56	0.15	0.57
(2,822)	1:73:B:ILE:HG23	1:11:B:LYS:HA	10	0.56	0.15	0.57
(2,822)	1:73:B:ILE:HG21	1:11:B:LYS:HA	10	0.56	0.15	0.57
(2,822)	1:73:B:ILE:HG23	1:75:B:SER:HA	10	0.56	0.15	0.57
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	10	0.56	0.01	0.56
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG23	10	0.56	0.11	0.59
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	10	0.56	0.11	0.59
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG22	10	0.56	0.11	0.59
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	10	0.56	0.03	0.56
(2,630)	1:15:B:LEU:HD11	1:15:B:LEU:HA	10	0.56	0.03	0.56
(2,630)	1:15:B:LEU:HD12	1:15:B:LEU:HA	10	0.56	0.03	0.56
(2,776)	1:31:B:ILE:HG22	1:40:B:PHE:HE1	10	0.56	0.23	0.52
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE2	10	0.56	0.23	0.52
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE1	10	0.56	0.23	0.52
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE1	10	0.56	0.23	0.52
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE2	10	0.56	0.23	0.52
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	10	0.55	0.14	0.52
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	10	0.55	0.18	0.54
(2,514)	1:22:B:LEU:HD23	1:82:B:GLY:HA3	10	0.55	0.18	0.54
(2,514)	1:22:B:LEU:HD22	1:82:B:GLY:HA3	10	0.55	0.18	0.54
(2,801)	1:89:B:ILE:HD12	1:86:B:GLY:HA3	10	0.55	0.14	0.58
(2,801)	1:89:B:ILE:HD11	1:86:B:GLY:HA3	10	0.55	0.14	0.58
(2,801)	1:89:B:ILE:HD13	1:86:B:GLY:HA3	10	0.55	0.14	0.58
(2,810)	1:58:B:THR:H	1:89:B:ILE:HD11	10	0.55	0.06	0.57
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG21	10	0.55	0.06	0.57
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG22	10	0.55	0.06	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG23	10	0.55	0.06	0.57
(2,810)	1:89:B:ILE:H	1:89:B:ILE:HD11	10	0.55	0.06	0.57
(2,810)	1:89:B:ILE:H	1:89:B:ILE:HD12	10	0.55	0.06	0.57
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG11	10	0.55	0.06	0.55
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	10	0.55	0.06	0.55
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG13	10	0.55	0.06	0.55
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD12	10	0.55	0.09	0.52
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD11	10	0.55	0.09	0.52
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD13	10	0.55	0.09	0.52
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	10	0.54	0.1	0.56
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	10	0.54	0.13	0.55
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE2	10	0.54	0.13	0.55
(2,391)	1:48:B:GLU:HB3	1:47:B:TYR:HD1	10	0.54	0.13	0.55
(2,391)	1:48:B:GLU:HB3	1:47:B:TYR:HD2	10	0.54	0.13	0.55
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	10	0.53	0.01	0.54
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	10	0.52	0.14	0.5
(2,888)	1:73:B:ILE:H	1:73:B:ILE:HD11	10	0.52	0.08	0.55
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE3	10	0.52	0.08	0.55
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE2	10	0.52	0.08	0.55
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE1	10	0.52	0.08	0.55
(2,888)	1:73:B:ILE:H	1:73:B:ILE:HD12	10	0.52	0.08	0.55
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	10	0.52	0.08	0.54
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG21	10	0.52	0.02	0.52
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG22	10	0.52	0.02	0.52
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG23	10	0.52	0.02	0.52
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	10	0.52	0.13	0.48
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE1	10	0.52	0.13	0.48
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	10	0.52	0.39	0.25
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD23	10	0.52	0.39	0.25
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	10	0.52	0.39	0.25
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG21	10	0.52	0.14	0.51
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG22	10	0.52	0.14	0.51
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG23	10	0.52	0.14	0.51
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	10	0.52	0.01	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD23	10	0.52	0.01	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD21	10	0.52	0.01	0.52
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	10	0.51	0.01	0.51
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	10	0.51	0.01	0.51
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	10	0.51	0.1	0.53
(2,778)	1:31:B:ILE:HG23	1:32:B:GLN:HG3	10	0.51	0.15	0.51
(2,778)	1:31:B:ILE:HG21	1:32:B:GLN:HG3	10	0.51	0.15	0.51
(2,778)	1:31:B:ILE:HG22	1:32:B:GLN:HG3	10	0.51	0.15	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,778)	1:99:B:ILE:HG23	1:95:B:GLU:HG2	10	0.51	0.15	0.51
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	10	0.51	0.16	0.58
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	10	0.51	0.14	0.51
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD1	10	0.5	0.16	0.57
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD2	10	0.5	0.16	0.57
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	10	0.5	0.16	0.57
(2,772)	1:13:B:ALA:HB2	1:16:B:ASN:HB3	10	0.5	0.05	0.51
(2,772)	1:13:B:ALA:HB3	1:16:B:ASN:HB3	10	0.5	0.05	0.51
(2,772)	1:13:B:ALA:HB1	1:16:B:ASN:HB3	10	0.5	0.05	0.51
(2,772)	1:67:B:ALA:HB3	1:66:B:TYR:HB3	10	0.5	0.05	0.51
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	10	0.5	0.03	0.5
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	10	0.49	0.08	0.48
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	10	0.49	0.08	0.48
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD13	10	0.49	0.08	0.48
(2,964)	1:7:B:ASN:HB3	1:8:B:GLU:HG2	10	0.49	0.14	0.52
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	10	0.49	0.14	0.52
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	10	0.49	0.03	0.5
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG21	10	0.49	0.03	0.5
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG22	10	0.49	0.03	0.5
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	10	0.49	0.09	0.52
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE2	10	0.48	0.09	0.52
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE1	10	0.48	0.09	0.52
(2,1313)	1:66:B:TYR:H	1:66:B:TYR:HD2	10	0.48	0.09	0.52
(2,1313)	1:66:B:TYR:H	1:69:B:MET:H	10	0.48	0.09	0.52
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	10	0.48	0.11	0.46
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD13	10	0.48	0.11	0.46
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG22	10	0.47	0.02	0.48
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG23	10	0.47	0.02	0.48
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	10	0.47	0.02	0.48
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB2	10	0.47	0.09	0.45
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB3	10	0.47	0.09	0.45
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB1	10	0.47	0.09	0.45
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	10	0.47	0.05	0.45
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	10	0.47	0.05	0.48
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	10	0.47	0.06	0.46
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	10	0.47	0.01	0.47
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HZ3	10	0.46	0.14	0.49
(2,1157)	1:73:B:ILE:HG23	1:14:B:TRP:HZ3	10	0.46	0.14	0.49
(2,1157)	1:73:B:ILE:HG21	1:14:B:TRP:HZ3	10	0.46	0.14	0.49
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HH2	10	0.46	0.14	0.49
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	10	0.46	0.03	0.46
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD13	10	0.46	0.1	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,890)	1:11:B:LYS:H	1:69:B:MET:HE2	10	0.46	0.1	0.46
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD11	10	0.46	0.1	0.46
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD12	10	0.46	0.1	0.46
(2,890)	1:11:B:LYS:H	1:69:B:MET:HE3	10	0.46	0.1	0.46
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	10	0.46	0.11	0.43
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD21	10	0.46	0.11	0.43
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD23	10	0.46	0.11	0.43
(1,812)	1:80:B:THR:HG22	1:81:B:TRP:HZ2	10	0.45	0.19	0.47
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	10	0.45	0.19	0.47
(1,812)	1:80:B:THR:HG21	1:81:B:TRP:HZ2	10	0.45	0.19	0.47
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	10	0.45	0.11	0.46
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG23	10	0.45	0.11	0.46
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG21	10	0.45	0.11	0.46
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB2	10	0.45	0.08	0.46
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB3	10	0.45	0.08	0.46
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB1	10	0.45	0.08	0.46
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	10	0.45	0.12	0.47
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	10	0.45	0.16	0.4
(2,859)	1:51:B:VAL:HG13	1:23:B:PRO:HD2	10	0.45	0.04	0.44
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	10	0.45	0.04	0.44
(2,859)	1:51:B:VAL:HG11	1:23:B:PRO:HD2	10	0.45	0.04	0.44
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	10	0.45	0.01	0.45
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	10	0.45	0.13	0.48
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	10	0.45	0.04	0.45
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	10	0.45	0.04	0.45
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	10	0.45	0.04	0.45
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	10	0.44	0.19	0.36
(2,973)	1:76:B:GLU:HG2	1:80:B:THR:HB	10	0.44	0.19	0.36
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB2	10	0.44	0.19	0.36
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	10	0.44	0.05	0.44
(2,762)	1:13:B:ALA:HB3	1:14:B:TRP:HB2	10	0.44	0.08	0.44
(2,762)	1:13:B:ALA:HB1	1:14:B:TRP:HB2	10	0.44	0.08	0.44
(2,762)	1:13:B:ALA:HB2	1:14:B:TRP:HB2	10	0.44	0.08	0.44
(2,762)	1:9:B:MET:HE1	1:14:B:TRP:HB2	10	0.44	0.08	0.44
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	10	0.44	0.11	0.46
(2,480)	1:85:B:LEU:HG	1:89:B:ILE:H	10	0.44	0.11	0.46
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	10	0.44	0.11	0.47
(2,1066)	1:101:B:LYS:H	1:99:B:ILE:HG13	10	0.44	0.11	0.47
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	10	0.43	0.05	0.44
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD23	10	0.43	0.06	0.44
(2,1099)	1:22:B:LEU:H	1:22:B:LEU:HD12	10	0.43	0.06	0.44
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD21	10	0.43	0.06	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1099)	1:22:B:LEU:H	1:22:B:LEU:HD13	10	0.43	0.06	0.44
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD22	10	0.43	0.06	0.44
(2,1078)	1:65:B:LEU:HD13	1:88:B:CYS:H	10	0.42	0.11	0.42
(2,1078)	1:65:B:LEU:HD12	1:88:B:CYS:H	10	0.42	0.11	0.42
(2,1078)	1:65:B:LEU:HD11	1:88:B:CYS:H	10	0.42	0.11	0.42
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	10	0.42	0.15	0.41
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD21	10	0.42	0.15	0.41
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD22	10	0.42	0.15	0.41
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB3	10	0.42	0.06	0.4
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	0.42	0.06	0.4
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB2	10	0.42	0.06	0.4
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	10	0.41	0.06	0.42
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	10	0.41	0.02	0.4
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	10	0.41	0.01	0.41
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	10	0.4	0.04	0.39
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG23	10	0.4	0.13	0.38
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	10	0.4	0.13	0.38
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG22	10	0.4	0.13	0.38
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD11	10	0.4	0.12	0.39
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	10	0.4	0.12	0.39
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD12	10	0.4	0.12	0.39
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	10	0.39	0.09	0.39
(2,889)	1:73:B:ILE:HD13	1:78:B:ALA:H	10	0.39	0.09	0.39
(2,889)	1:73:B:ILE:HD11	1:78:B:ALA:H	10	0.39	0.09	0.39
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	10	0.39	0.07	0.36
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB2	10	0.39	0.09	0.37
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB3	10	0.39	0.09	0.37
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB1	10	0.39	0.09	0.37
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG22	10	0.38	0.05	0.41
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG23	10	0.38	0.05	0.41
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	10	0.38	0.05	0.41
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	10	0.38	0.09	0.36
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	10	0.38	0.01	0.38
(2,877)	1:89:B:ILE:H	1:86:B:GLY:HA2	10	0.38	0.01	0.38
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB2	10	0.37	0.09	0.4
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB3	10	0.37	0.09	0.4
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB1	10	0.37	0.09	0.4
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	10	0.37	0.25	0.26
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE1	10	0.37	0.25	0.26
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE3	10	0.37	0.25	0.26
(2,900)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	10	0.37	0.25	0.26
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	10	0.37	0.19	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,565)	1:15:B:LEU:HD21	1:62:B:GLN:HA	10	0.37	0.19	0.3
(2,565)	1:15:B:LEU:HD22	1:62:B:GLN:HA	10	0.37	0.19	0.3
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	10	0.36	0.11	0.36
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB3	10	0.36	0.11	0.36
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD11	10	0.36	0.01	0.36
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD13	10	0.36	0.01	0.36
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD12	10	0.36	0.01	0.36
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	10	0.36	0.02	0.37
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	10	0.36	0.08	0.36
(2,374)	1:23:B:PRO:HG2	1:55:B:PRO:HB3	10	0.36	0.08	0.36
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	10	0.36	0.1	0.36
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB1	10	0.35	0.06	0.35
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB2	10	0.35	0.06	0.35
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB3	10	0.35	0.06	0.35
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	10	0.35	0.18	0.32
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD21	10	0.35	0.18	0.32
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD23	10	0.35	0.18	0.32
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	10	0.34	0.02	0.34
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG23	10	0.34	0.12	0.32
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG21	10	0.34	0.12	0.32
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	10	0.34	0.12	0.32
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	10	0.34	0.07	0.36
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	10	0.34	0.0	0.34
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.34	0.03	0.34
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	10	0.34	0.05	0.36
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD12	10	0.34	0.05	0.36
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD13	10	0.34	0.05	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD12	10	0.34	0.08	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD11	10	0.34	0.08	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD13	10	0.34	0.08	0.36
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	10	0.33	0.11	0.34
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG22	10	0.33	0.15	0.31
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	10	0.33	0.15	0.31
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG21	10	0.33	0.15	0.31
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB3	10	0.33	0.08	0.32
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB1	10	0.33	0.08	0.32
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB2	10	0.33	0.08	0.32
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	10	0.33	0.08	0.34
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	10	0.33	0.1	0.32
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	10	0.33	0.09	0.32
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	10	0.32	0.05	0.32
(2,596)	1:61:B:CYS:H	1:60:B:LYS:HG3	10	0.32	0.09	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	10	0.32	0.09	0.35
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	10	0.32	0.08	0.3
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	10	0.32	0.03	0.31
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB3	10	0.32	0.08	0.3
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	10	0.32	0.08	0.3
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	10	0.32	0.08	0.3
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	10	0.31	0.01	0.31
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	10	0.31	0.07	0.34
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	10	0.31	0.1	0.26
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	10	0.31	0.03	0.3
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	10	0.3	0.01	0.3
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG23	10	0.3	0.02	0.3
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	10	0.3	0.02	0.3
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG21	10	0.3	0.02	0.3
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.3	0.03	0.3
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG21	10	0.3	0.06	0.3
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	10	0.3	0.06	0.3
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG22	10	0.3	0.06	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	10	0.29	0.01	0.3
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	10	0.29	0.01	0.3
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	10	0.29	0.06	0.3
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB3	10	0.29	0.06	0.3
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	10	0.29	0.04	0.29
(2,969)	1:76:B:GLU:HG2	1:80:B:THR:H	10	0.29	0.04	0.29
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	10	0.29	0.03	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	10	0.28	0.0	0.28
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG22	10	0.28	0.06	0.3
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	10	0.28	0.06	0.3
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG23	10	0.28	0.06	0.3
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD11	10	0.27	0.06	0.26
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD13	10	0.27	0.06	0.26
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	10	0.27	0.06	0.26
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD11	10	0.27	0.03	0.28
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD13	10	0.27	0.03	0.28
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	10	0.27	0.03	0.28
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	10	0.27	0.06	0.26
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB3	10	0.27	0.06	0.26
(2,608)	1:85:B:LEU:HD23	1:62:B:GLN:HB2	10	0.27	0.16	0.24
(2,608)	1:85:B:LEU:HD22	1:62:B:GLN:HB2	10	0.27	0.16	0.24
(2,608)	1:85:B:LEU:HD21	1:62:B:GLN:HB2	10	0.27	0.16	0.24
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	10	0.27	0.02	0.26
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	10	0.26	0.03	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	10	0.26	0.05	0.26
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	10	0.26	0.01	0.26
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG22	10	0.26	0.01	0.26
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG23	10	0.26	0.01	0.26
(2,42)	1:28:B:LYS:H	1:28:B:LYS:HE3	10	0.25	0.08	0.24
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	10	0.25	0.08	0.24
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	10	0.25	0.01	0.25
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	10	0.25	0.06	0.25
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	10	0.25	0.03	0.26
(2,128)	1:40:B:PHE:HB2	1:36:B:LEU:HA	10	0.25	0.17	0.22
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	10	0.25	0.17	0.22
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	10	0.24	0.11	0.21
(2,687)	1:38:B:LYS:HA	1:41:B:ASP:H	10	0.24	0.11	0.21
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD21	10	0.24	0.05	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	10	0.24	0.05	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD22	10	0.24	0.05	0.24
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG23	10	0.24	0.03	0.24
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG21	10	0.24	0.03	0.24
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG22	10	0.24	0.03	0.24
(2,713)	1:51:B:VAL:HG13	1:24:B:ASP:HA	10	0.23	0.09	0.2
(2,713)	1:51:B:VAL:HG12	1:24:B:ASP:HA	10	0.23	0.09	0.2
(2,713)	1:51:B:VAL:HG11	1:24:B:ASP:HA	10	0.23	0.09	0.2
(2,713)	1:51:B:VAL:HG22	1:52:B:THR:HB	10	0.23	0.09	0.2
(2,713)	1:51:B:VAL:HG21	1:52:B:THR:HB	10	0.23	0.09	0.2
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	10	0.23	0.0	0.23
(2,1434)	1:60:B:LYS:H	1:57:B:SER:HB3	10	0.23	0.07	0.22
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	10	0.23	0.07	0.22
(2,1434)	1:22:B:LEU:H	1:58:B:THR:HB	10	0.23	0.07	0.22
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	10	0.23	0.0	0.23
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD11	10	0.22	0.06	0.22
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD13	10	0.22	0.06	0.22
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	10	0.22	0.06	0.22
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	10	0.22	0.01	0.22
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	10	0.21	0.0	0.21
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	10	0.2	0.03	0.22
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB2	10	0.2	0.01	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	10	0.2	0.01	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB3	10	0.2	0.01	0.2
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	10	0.2	0.08	0.18
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG22	10	0.2	0.08	0.18
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG23	10	0.2	0.08	0.18
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	10	0.2	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	10	0.2	0.03	0.18
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	10	0.19	0.01	0.2
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	10	0.19	0.01	0.2
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	10	0.19	0.01	0.19
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	10	0.19	0.02	0.18
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	10	0.19	0.0	0.19
(1,809)	1:52:B:THR:HG21	1:52:B:THR:HB	10	0.19	0.0	0.19
(1,809)	1:52:B:THR:HG23	1:52:B:THR:HB	10	0.19	0.0	0.19
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG21	10	0.19	0.02	0.18
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG22	10	0.19	0.02	0.18
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG23	10	0.19	0.02	0.18
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	10	0.18	0.04	0.2
(2,257)	1:54:B:ILE:H	1:23:B:PRO:HB3	10	0.18	0.04	0.2
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB3	10	0.18	0.07	0.17
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	0.18	0.07	0.17
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB2	10	0.18	0.07	0.17
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	10	0.18	0.0	0.18
(2,244)	1:6:B:PRO:HB2	1:6:B:PRO:HA	10	0.18	0.0	0.18
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	10	0.18	0.04	0.18
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	10	0.18	0.02	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	10	0.18	0.0	0.18
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	10	0.17	0.04	0.16
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	10	0.17	0.01	0.16
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	10	0.15	0.01	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD12	10	0.15	0.01	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD13	10	0.15	0.01	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD11	10	0.15	0.01	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB3	10	0.15	0.01	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	10	0.15	0.01	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB1	10	0.15	0.01	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	10	0.14	0.0	0.15
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG23	10	0.14	0.01	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG21	10	0.14	0.01	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	10	0.14	0.01	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG22	10	0.14	0.0	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG23	10	0.14	0.0	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG21	10	0.14	0.0	0.14
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	10	0.13	0.01	0.14
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	10	0.13	0.01	0.14
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG23	10	0.12	0.01	0.12
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	10	0.12	0.01	0.12
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG21	10	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,582)	1:94:B:ALA:HB2	1:94:B:ALA:HA	10	0.11	0.01	0.11
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	10	0.11	0.01	0.11
(1,582)	1:94:B:ALA:HB1	1:94:B:ALA:HA	10	0.11	0.01	0.11
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	9	2.61	0.09	2.66
(2,1143)	1:4:B:ALA:HB3	1:5:B:ASN:HB3	9	1.45	0.57	1.25
(2,1143)	1:4:B:ALA:HB2	1:5:B:ASN:HB3	9	1.45	0.57	1.25
(2,1143)	1:4:B:ALA:HB1	1:5:B:ASN:HB3	9	1.45	0.57	1.25
(2,1143)	1:78:B:ALA:HB2	1:74:B:ASN:HB2	9	1.45	0.57	1.25
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD22	9	1.41	1.18	0.51
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	9	1.41	1.18	0.51
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD23	9	1.41	1.18	0.51
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	9	1.13	0.04	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD22	9	1.13	0.04	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD21	9	1.13	0.04	1.14
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	9	1.1	0.32	0.99
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD11	9	1.1	0.32	0.99
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	9	1.1	0.32	0.99
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	9	1.03	0.28	1.18
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	9	1.03	0.92	0.24
(1,500)	1:36:B:LEU:HD13	1:36:B:LEU:HA	9	1.03	0.92	0.24
(1,500)	1:36:B:LEU:HD11	1:36:B:LEU:HA	9	1.03	0.92	0.24
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD21	9	1.01	0.25	1.03
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD11	9	1.01	0.25	1.03
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD12	9	1.01	0.25	1.03
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD23	9	1.01	0.25	1.03
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD22	9	1.01	0.25	1.03
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	9	0.97	0.29	1.13
(2,117)	1:50:B:CYS:HB2	1:31:B:ILE:HD13	9	0.96	0.23	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD11	9	0.96	0.23	0.88
(2,117)	1:50:B:CYS:HB2	1:45:B:MET:HE3	9	0.96	0.23	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	9	0.96	0.23	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	9	0.96	0.23	0.88
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	9	0.9	0.27	0.94
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	9	0.9	0.18	0.9
(2,959)	1:88:B:CYS:HB2	1:89:B:ILE:HG13	9	0.9	0.18	0.9
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD21	9	0.88	0.09	0.85
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD22	9	0.88	0.09	0.85
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD23	9	0.88	0.09	0.85
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB3	9	0.81	0.12	0.82
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB1	9	0.81	0.12	0.82
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB2	9	0.81	0.12	0.82
(2,1121)	1:60:B:LYS:HD2	1:92:B:ASP:HA	9	0.81	0.12	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1304)	1:15:B:LEU:H	1:85:B:LEU:HD21	9	0.78	0.17	0.74
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	9	0.78	0.17	0.74
(2,1304)	1:15:B:LEU:H	1:85:B:LEU:HD23	9	0.78	0.17	0.74
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD23	9	0.77	0.14	0.76
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD21	9	0.77	0.14	0.76
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD22	9	0.77	0.14	0.76
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	9	0.76	0.17	0.72
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	9	0.75	0.09	0.8
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	9	0.74	0.0	0.74
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG23	9	0.7	0.26	0.76
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG22	9	0.7	0.26	0.76
(2,1159)	1:28:B:LYS:HB2	1:31:B:ILE:HD12	9	0.7	0.26	0.76
(2,1159)	1:45:B:MET:HG3	1:43:B:ILE:HG22	9	0.7	0.26	0.76
(2,1159)	1:45:B:MET:HG3	1:43:B:ILE:HG21	9	0.7	0.26	0.76
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	9	0.69	0.25	0.78
(2,4)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	9	0.69	0.25	0.78
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	9	0.68	0.19	0.65
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	9	0.67	0.4	0.5
(2,409)	1:97:B:HIS:HB3	1:96:B:LYS:HD3	9	0.67	0.4	0.5
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD2	9	0.67	0.4	0.5
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	9	0.66	0.02	0.65
(2,1502)	1:38:B:LYS:H	1:38:B:LYS:HD2	9	0.66	0.02	0.65
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB2	9	0.66	0.25	0.69
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	9	0.66	0.25	0.69
(2,1094)	1:69:B:MET:HB2	1:70:B:PRO:HA	9	0.66	0.25	0.69
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB1	9	0.66	0.25	0.69
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	9	0.65	0.3	0.71
(2,1058)	1:44:B:LYS:HD3	1:41:B:ASP:HB3	9	0.65	0.3	0.71
(2,1058)	1:92:B:ASP:HB2	1:91:B:LYS:HD3	9	0.65	0.3	0.71
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD13	9	0.64	0.65	0.4
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD11	9	0.64	0.65	0.4
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD12	9	0.64	0.65	0.4
(2,46)	1:61:B:CYS:HB3	1:89:B:ILE:HD13	9	0.63	0.13	0.63
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	9	0.63	0.13	0.63
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG23	9	0.63	0.13	0.63
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG21	9	0.63	0.13	0.63
(2,761)	1:13:B:ALA:HB3	1:9:B:MET:HA	9	0.63	0.24	0.76
(2,761)	1:9:B:MET:HE1	1:9:B:MET:HA	9	0.63	0.24	0.76
(2,761)	1:13:B:ALA:HB2	1:9:B:MET:HA	9	0.63	0.24	0.76
(2,761)	1:13:B:ALA:HB1	1:9:B:MET:HA	9	0.63	0.24	0.76
(2,761)	1:9:B:MET:HE3	1:9:B:MET:HA	9	0.63	0.24	0.76
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	9	0.62	0.21	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,948)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	9	0.62	0.21	0.57
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD23	9	0.62	0.1	0.63
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD12	9	0.62	0.1	0.63
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD11	9	0.62	0.1	0.63
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD13	9	0.62	0.1	0.63
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD22	9	0.62	0.1	0.63
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD21	9	0.62	0.1	0.63
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	9	0.61	0.05	0.61
(2,1359)	1:58:B:THR:H	1:59:B:LYS:HG3	9	0.61	0.05	0.61
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	9	0.61	0.22	0.63
(2,1474)	1:63:B:ASP:H	1:59:B:LYS:HD3	9	0.61	0.22	0.63
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	9	0.61	0.18	0.7
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE1	9	0.61	0.18	0.7
(2,715)	1:51:B:VAL:HG12	1:27:B:CYS:HB3	9	0.59	0.26	0.67
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	9	0.59	0.26	0.67
(2,715)	1:51:B:VAL:HG13	1:27:B:CYS:HB3	9	0.59	0.26	0.67
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	9	0.58	0.52	0.45
(2,1084)	1:53:B:LEU:HD13	1:96:B:LYS:HD3	9	0.58	0.52	0.45
(2,1084)	1:53:B:LEU:HD11	1:96:B:LYS:HD3	9	0.58	0.52	0.45
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	9	0.55	0.39	0.44
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB3	9	0.55	0.07	0.57
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	9	0.55	0.07	0.57
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB1	9	0.55	0.07	0.57
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	9	0.53	0.22	0.53
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD11	9	0.53	0.22	0.53
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	9	0.53	0.22	0.53
(2,131)	1:40:B:PHE:HB2	1:45:B:MET:HE2	9	0.53	0.22	0.53
(2,131)	1:40:B:PHE:HB2	1:45:B:MET:HE1	9	0.53	0.22	0.53
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	9	0.52	0.12	0.55
(2,545)	1:17:B:SER:HB3	1:14:B:TRP:HD1	9	0.52	0.12	0.55
(2,556)	1:45:B:MET:HE3	1:98:B:LEU:HA	9	0.5	0.2	0.53
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	9	0.5	0.2	0.53
(2,556)	1:45:B:MET:HE2	1:45:B:MET:HA	9	0.5	0.2	0.53
(2,556)	1:45:B:MET:HE2	1:98:B:LEU:HA	9	0.5	0.2	0.53
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	9	0.49	0.18	0.44
(2,57)	1:85:B:LEU:HB3	1:19:B:THR:HA	9	0.49	0.18	0.44
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG22	9	0.49	0.16	0.48
(2,1045)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	9	0.49	0.16	0.48
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	9	0.49	0.16	0.48
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG21	9	0.49	0.16	0.48
(2,1045)	1:23:B:PRO:HG2	1:54:B:ILE:HG22	9	0.49	0.16	0.48
(1,598)	1:26:B:ILE:HG21	1:90:B:GLY:HA3	9	0.48	0.13	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,598)	1:26:B:ILE:HG22	1:90:B:GLY:HA3	9	0.48	0.13	0.54
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	9	0.48	0.13	0.54
(2,1117)	1:-6:B:VAL:HG12	1:-4:B:ASP:H	9	0.48	0.34	0.41
(2,1117)	1:-6:B:VAL:HG11	1:-4:B:ASP:H	9	0.48	0.34	0.41
(2,1117)	1:-6:B:VAL:HG22	1:-4:B:ASP:H	9	0.48	0.34	0.41
(2,1117)	1:-6:B:VAL:HG21	1:-4:B:ASP:H	9	0.48	0.34	0.41
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	9	0.47	0.17	0.46
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HD1	9	0.47	0.17	0.46
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HD2	9	0.47	0.17	0.46
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	9	0.47	0.19	0.51
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE2	9	0.47	0.19	0.51
(2,1029)	1:44:B:LYS:HD2	1:43:B:ILE:HA	9	0.47	0.07	0.48
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	9	0.47	0.07	0.48
(2,802)	1:26:B:ILE:HG21	1:86:B:GLY:HA2	9	0.47	0.21	0.47
(2,802)	1:26:B:ILE:HG22	1:86:B:GLY:HA2	9	0.47	0.21	0.47
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	9	0.47	0.21	0.47
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	9	0.47	0.25	0.44
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	9	0.47	0.21	0.42
(2,453)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	9	0.47	0.21	0.42
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	9	0.45	0.08	0.48
(2,39)	1:33:B:ASP:HB2	1:36:B:LEU:HD22	9	0.45	0.14	0.47
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD12	9	0.45	0.14	0.47
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD11	9	0.45	0.14	0.47
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	9	0.45	0.14	0.47
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	9	0.45	0.03	0.45
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD22	9	0.44	0.31	0.37
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD23	9	0.44	0.31	0.37
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD21	9	0.44	0.31	0.37
(2,220)	1:18:B:MET:HE3	1:18:B:MET:HB3	9	0.44	0.31	0.37
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG23	9	0.43	0.17	0.43
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG22	9	0.43	0.17	0.43
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG21	9	0.43	0.17	0.43
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	9	0.43	0.03	0.44
(2,1362)	1:11:B:LYS:H	1:11:B:LYS:HB2	9	0.43	0.03	0.44
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	9	0.42	0.0	0.42
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	9	0.41	0.08	0.4
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD23	9	0.41	0.08	0.4
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD21	9	0.41	0.08	0.4
(2,606)	1:85:B:LEU:HD21	1:66:B:TYR:H	9	0.41	0.18	0.46
(2,606)	1:85:B:LEU:HD23	1:66:B:TYR:H	9	0.41	0.18	0.46
(2,606)	1:86:B:GLY:H	1:85:B:LEU:HD22	9	0.41	0.18	0.46
(2,606)	1:85:B:LEU:HD22	1:66:B:TYR:H	9	0.41	0.18	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	9	0.4	0.08	0.43
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	9	0.4	0.09	0.37
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	9	0.38	0.1	0.4
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	9	0.36	0.11	0.37
(2,694)	1:42:B:GLU:HA	1:42:B:GLU:HG3	9	0.36	0.11	0.37
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	9	0.36	0.14	0.44
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	9	0.35	0.0	0.35
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	9	0.34	0.11	0.36
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	9	0.33	0.12	0.34
(2,1538)	1:72:B:LYS:H	1:70:B:PRO:HG3	9	0.33	0.12	0.34
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	9	0.33	0.01	0.33
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	9	0.32	0.04	0.31
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	9	0.31	0.12	0.32
(2,45)	1:61:B:CYS:HB3	1:65:B:LEU:HG	9	0.31	0.12	0.32
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD13	9	0.3	0.11	0.27
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD12	9	0.3	0.11	0.27
(2,1458)	1:93:B:PHE:H	1:26:B:ILE:HG22	9	0.3	0.11	0.27
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD11	9	0.3	0.11	0.27
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	9	0.3	0.21	0.19
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	9	0.29	0.02	0.28
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD12	9	0.29	0.26	0.21
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD22	9	0.29	0.26	0.21
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD13	9	0.29	0.26	0.21
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD11	9	0.29	0.26	0.21
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD21	9	0.28	0.16	0.22
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD22	9	0.28	0.16	0.22
(2,5)	1:65:B:LEU:HB2	1:85:B:LEU:HD12	9	0.28	0.16	0.22
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD23	9	0.28	0.16	0.22
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HE2	9	0.28	0.06	0.27
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD2	9	0.28	0.06	0.27
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD1	9	0.28	0.06	0.27
(1,811)	1:18:B:MET:H	1:19:B:THR:HG22	9	0.26	0.04	0.28
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	9	0.26	0.04	0.28
(1,811)	1:18:B:MET:H	1:19:B:THR:HG23	9	0.26	0.04	0.28
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD11	9	0.26	0.06	0.27
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD12	9	0.26	0.06	0.27
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD23	9	0.26	0.06	0.27
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD13	9	0.26	0.06	0.27
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD21	9	0.26	0.06	0.27
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	9	0.26	0.12	0.23
(2,47)	1:87:B:GLU:H	1:85:B:LEU:HB3	9	0.26	0.12	0.23
(2,1392)	1:88:B:CYS:H	1:89:B:ILE:HG12	9	0.26	0.07	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD13	9	0.26	0.07	0.27
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD12	9	0.26	0.07	0.27
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD11	9	0.26	0.07	0.27
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	9	0.26	0.08	0.29
(2,858)	1:58:B:THR:HG23	1:23:B:PRO:HD2	9	0.26	0.08	0.29
(2,858)	1:58:B:THR:HG22	1:23:B:PRO:HD2	9	0.26	0.08	0.29
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HD1	9	0.25	0.04	0.24
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	9	0.25	0.04	0.24
(2,1163)	1:54:B:ILE:HD11	1:23:B:PRO:HG3	9	0.24	0.07	0.25
(2,1163)	1:54:B:ILE:HD13	1:23:B:PRO:HG3	9	0.24	0.07	0.25
(2,1163)	1:54:B:ILE:HD12	1:23:B:PRO:HG3	9	0.24	0.07	0.25
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	9	0.24	0.03	0.26
(2,1112)	1:37:B:LYS:HD3	1:37:B:LYS:HA	9	0.24	0.03	0.26
(2,640)	1:-6:B:VAL:HA	1:-5:B:ASP:HA	9	0.22	0.06	0.2
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	9	0.22	0.06	0.2
(2,640)	1:40:B:PHE:HA	1:98:B:LEU:HA	9	0.22	0.06	0.2
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	9	0.21	0.05	0.23
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	9	0.2	0.02	0.18
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	9	0.18	0.05	0.15
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE2	9	0.18	0.05	0.15
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	9	0.18	0.04	0.17
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	9	0.16	0.03	0.17
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG21	9	0.14	0.01	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG23	9	0.14	0.01	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG22	9	0.14	0.01	0.15
(1,477)	1:98:B:LEU:HD23	1:93:B:PHE:HE2	9	0.14	0.02	0.13
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE1	9	0.14	0.02	0.13
(1,477)	1:98:B:LEU:HD21	1:93:B:PHE:HE2	9	0.14	0.02	0.13
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE2	9	0.14	0.02	0.13
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	9	0.11	0.0	0.11
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	9	0.1	0.0	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD11	9	0.1	0.0	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD12	9	0.1	0.0	0.1
(2,1044)	1:95:B:GLU:HB2	1:99:B:ILE:HD13	8	0.86	0.55	1.1
(2,1044)	1:95:B:GLU:HB2	1:99:B:ILE:HD11	8	0.86	0.55	1.1
(2,1044)	1:95:B:GLU:HB2	1:96:B:LYS:HB2	8	0.86	0.55	1.1
(2,1044)	1:32:B:GLN:HB2	1:31:B:ILE:HG21	8	0.86	0.55	1.1
(2,1044)	1:32:B:GLN:HB2	1:31:B:ILE:HG22	8	0.86	0.55	1.1
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	8	0.68	0.11	0.7
(2,341)	1:38:B:LYS:HD2	1:38:B:LYS:HA	8	0.68	0.11	0.7
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	8	0.6	0.24	0.56
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	8	0.58	0.07	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	8	0.57	0.27	0.52
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	8	0.57	0.04	0.56
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	8	0.54	0.09	0.55
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE1	8	0.52	0.04	0.54
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE2	8	0.52	0.04	0.54
(2,956)	1:50:B:CYS:HB2	1:40:B:PHE:HE2	8	0.52	0.04	0.54
(2,956)	1:50:B:CYS:HB2	1:93:B:PHE:HE1	8	0.52	0.04	0.54
(2,956)	1:50:B:CYS:HB2	1:40:B:PHE:HE1	8	0.52	0.04	0.54
(2,956)	1:50:B:CYS:HB2	1:47:B:TYR:HD1	8	0.52	0.04	0.54
(2,985)	1:62:B:GLN:HG3	1:59:B:LYS:HD3	8	0.51	0.15	0.49
(2,985)	1:32:B:GLN:HG2	1:28:B:LYS:HD3	8	0.51	0.15	0.49
(2,985)	1:62:B:GLN:HG2	1:59:B:LYS:HD3	8	0.51	0.15	0.49
(2,985)	1:32:B:GLN:HG2	1:28:B:LYS:HD2	8	0.51	0.15	0.49
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE2	8	0.51	0.33	0.34
(2,688)	1:38:B:LYS:HA	1:38:B:LYS:HE3	8	0.51	0.33	0.34
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE3	8	0.51	0.33	0.34
(2,688)	1:38:B:LYS:HA	1:38:B:LYS:HE2	8	0.51	0.33	0.34
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	8	0.5	0.16	0.52
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	8	0.5	0.15	0.55
(2,1422)	1:41:B:ASP:H	1:44:B:LYS:HG3	8	0.5	0.15	0.55
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	8	0.5	0.38	0.36
(2,561)	1:22:B:LEU:HD21	1:14:B:TRP:HZ2	8	0.5	0.38	0.36
(2,561)	1:85:B:LEU:HD13	1:14:B:TRP:HZ2	8	0.5	0.38	0.36
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	8	0.43	0.05	0.46
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE3	8	0.42	0.11	0.42
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE1	8	0.42	0.11	0.42
(2,566)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	8	0.42	0.11	0.42
(2,566)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	8	0.42	0.11	0.42
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE2	8	0.42	0.11	0.42
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB3	8	0.42	0.17	0.42
(2,1142)	1:9:B:MET:HG3	1:78:B:ALA:HB1	8	0.42	0.17	0.42
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB2	8	0.42	0.17	0.42
(2,1142)	1:9:B:MET:HG3	1:78:B:ALA:HB2	8	0.42	0.17	0.42
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG2	8	0.41	0.13	0.4
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	8	0.41	0.13	0.4
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	8	0.4	0.22	0.3
(2,583)	1:21:B:LEU:HD11	1:17:B:SER:HB3	8	0.4	0.22	0.3
(2,583)	1:21:B:LEU:HD13	1:17:B:SER:HB3	8	0.4	0.22	0.3
(2,1415)	1:41:B:ASP:H	1:45:B:MET:HB2	8	0.39	0.16	0.35
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	8	0.39	0.16	0.35
(2,249)	1:100:B:PRO:HB3	1:43:B:ILE:HG21	8	0.39	0.12	0.42
(2,249)	1:100:B:PRO:HB3	1:43:B:ILE:HG23	8	0.39	0.12	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG23	8	0.39	0.12	0.42
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG21	8	0.39	0.12	0.42
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG22	8	0.39	0.12	0.42
(2,874)	1:26:B:ILE:HD11	1:90:B:GLY:HA3	8	0.35	0.16	0.36
(2,874)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	8	0.35	0.16	0.36
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	8	0.35	0.07	0.36
(2,666)	1:22:B:LEU:HD13	1:86:B:GLY:HA2	8	0.35	0.04	0.36
(2,666)	1:22:B:LEU:HD11	1:86:B:GLY:HA2	8	0.35	0.04	0.36
(2,666)	1:22:B:LEU:HD12	1:22:B:LEU:HA	8	0.35	0.04	0.36
(2,666)	1:22:B:LEU:HD13	1:22:B:LEU:HA	8	0.35	0.04	0.36
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD13	8	0.34	0.08	0.35
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD12	8	0.34	0.08	0.35
(2,1153)	1:27:B:CYS:H	1:54:B:ILE:HG23	8	0.34	0.08	0.35
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD11	8	0.34	0.08	0.35
(2,1153)	1:27:B:CYS:H	1:54:B:ILE:HG22	8	0.34	0.08	0.35
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG3	8	0.34	0.19	0.28
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG2	8	0.34	0.19	0.28
(2,996)	1:77:B:THR:HG23	1:70:B:PRO:HB3	8	0.34	0.19	0.28
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	8	0.34	0.1	0.31
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	8	0.32	0.01	0.32
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	8	0.32	0.07	0.31
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG23	8	0.32	0.14	0.29
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG22	8	0.32	0.14	0.29
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG21	8	0.32	0.14	0.29
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	8	0.3	0.11	0.32
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG23	8	0.29	0.14	0.29
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG22	8	0.29	0.14	0.29
(2,789)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	8	0.29	0.14	0.29
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG21	8	0.29	0.14	0.29
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	8	0.29	0.02	0.28
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG23	8	0.26	0.05	0.27
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG21	8	0.26	0.05	0.27
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG22	8	0.26	0.05	0.27
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG21	8	0.26	0.05	0.27
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	8	0.25	0.15	0.2
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD2	8	0.25	0.15	0.2
(2,1095)	1:15:B:LEU:HD12	1:66:B:TYR:H	8	0.25	0.09	0.24
(2,1095)	1:15:B:LEU:HD13	1:66:B:TYR:H	8	0.25	0.09	0.24
(2,1095)	1:12:B:ASP:H	1:15:B:LEU:HD13	8	0.25	0.09	0.24
(2,1095)	1:12:B:ASP:H	1:15:B:LEU:HD11	8	0.25	0.09	0.24
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG23	8	0.24	0.07	0.23
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG22	8	0.24	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG21	8	0.24	0.07	0.23
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	8	0.23	0.02	0.24
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	8	0.22	0.06	0.22
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	8	0.21	0.0	0.21
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	8	0.19	0.06	0.18
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB3	8	0.18	0.04	0.18
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB1	8	0.18	0.04	0.18
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB2	8	0.18	0.04	0.18
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	8	0.17	0.06	0.16
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	8	0.17	0.04	0.16
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	8	0.16	0.03	0.16
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	8	0.15	0.01	0.15
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	8	0.13	0.01	0.13
(2,717)	1:65:B:LEU:H	1:64:B:GLU:HA	8	0.13	0.01	0.13
(1,612)	1:78:B:ALA:HB3	1:78:B:ALA:HA	8	0.1	0.0	0.1
(1,612)	1:78:B:ALA:HB1	1:78:B:ALA:HA	8	0.1	0.0	0.1
(1,612)	1:78:B:ALA:HB2	1:78:B:ALA:HA	8	0.1	0.0	0.1
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	7	1.28	0.09	1.25
(2,1382)	1:30:B:PHE:H	1:26:B:ILE:HG12	7	1.28	0.09	1.25
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	7	0.9	0.33	0.92
(2,87)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	7	0.9	0.33	0.92
(2,87)	1:74:B:ASN:HB3	1:8:B:GLU:HB3	7	0.9	0.33	0.92
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	7	0.89	0.06	0.9
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	7	0.73	0.06	0.75
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE1	7	0.72	0.29	0.59
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE2	7	0.72	0.29	0.59
(2,1144)	1:17:B:SER:HB2	1:13:B:ALA:HB3	7	0.72	0.29	0.59
(2,1144)	1:17:B:SER:HB2	1:13:B:ALA:HB1	7	0.72	0.29	0.59
(2,905)	1:28:B:LYS:HG3	1:31:B:ILE:HD12	7	0.6	0.22	0.6
(2,905)	1:99:B:ILE:HD11	1:94:B:ALA:HB3	7	0.6	0.22	0.6
(2,905)	1:99:B:ILE:HD12	1:94:B:ALA:HB3	7	0.6	0.22	0.6
(2,905)	1:99:B:ILE:HD13	1:94:B:ALA:HB1	7	0.6	0.22	0.6
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	7	0.58	0.21	0.64
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	7	0.49	0.04	0.49
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	7	0.48	0.38	0.31
(2,104)	1:30:B:PHE:HB3	1:40:B:PHE:HE2	7	0.44	0.17	0.37
(2,104)	1:30:B:PHE:HB3	1:93:B:PHE:HE1	7	0.44	0.17	0.37
(2,104)	1:30:B:PHE:HB3	1:30:B:PHE:HE1	7	0.44	0.17	0.37
(2,104)	1:30:B:PHE:HB3	1:93:B:PHE:HE2	7	0.44	0.17	0.37
(2,104)	1:30:B:PHE:HB3	1:40:B:PHE:HE1	7	0.44	0.17	0.37
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD12	7	0.42	0.23	0.48
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD11	7	0.42	0.23	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD13	7	0.42	0.23	0.48
(2,81)	1:71:B:ASP:HB2	1:72:B:LYS:HG3	7	0.42	0.12	0.43
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD11	7	0.42	0.12	0.43
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD13	7	0.42	0.12	0.43
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	7	0.4	0.2	0.42
(2,1658)	1:77:B:THR:H	1:70:B:PRO:HG2	7	0.4	0.2	0.42
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	7	0.35	0.06	0.33
(2,1275)	1:62:B:GLN:H	1:59:B:LYS:HD3	7	0.35	0.06	0.33
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	7	0.35	0.13	0.33
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	7	0.34	0.1	0.36
(2,572)	1:26:B:ILE:HA	1:30:B:PHE:HD2	7	0.34	0.1	0.36
(2,96)	1:93:B:PHE:HB3	1:98:B:LEU:HD11	7	0.33	0.14	0.38
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG23	7	0.33	0.14	0.38
(2,96)	1:93:B:PHE:HB2	1:96:B:LYS:HB2	7	0.33	0.14	0.38
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG22	7	0.33	0.14	0.38
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG21	7	0.33	0.14	0.38
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	7	0.32	0.07	0.31
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG22	7	0.31	0.11	0.36
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG21	7	0.31	0.11	0.36
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG23	7	0.31	0.11	0.36
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG23	7	0.3	0.1	0.3
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG22	7	0.3	0.1	0.3
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG21	7	0.3	0.1	0.3
(2,430)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	7	0.3	0.17	0.21
(2,430)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	7	0.3	0.17	0.21
(2,430)	1:101:B:LYS:HD2	1:99:B:ILE:HG23	7	0.3	0.17	0.21
(2,430)	1:37:B:LYS:HD2	1:31:B:ILE:HG21	7	0.3	0.17	0.21
(2,430)	1:101:B:LYS:HD2	1:99:B:ILE:HG21	7	0.3	0.17	0.21
(2,332)	1:55:B:PRO:HG3	1:51:B:VAL:HA	7	0.29	0.11	0.27
(2,332)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	7	0.29	0.11	0.27
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD2	7	0.28	0.07	0.24
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD1	7	0.28	0.07	0.24
(2,164)	1:62:B:GLN:HG3	1:66:B:TYR:HD1	7	0.28	0.07	0.24
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	7	0.27	0.13	0.29
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD13	7	0.27	0.13	0.29
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD11	7	0.27	0.13	0.29
(2,188)	1:0:B:MET:HB3	1:-1:B:LYS:H	7	0.27	0.1	0.27
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	7	0.27	0.1	0.27
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE2	7	0.26	0.07	0.27
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE1	7	0.26	0.07	0.27
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE3	7	0.26	0.07	0.27
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	7	0.26	0.12	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	7	0.26	0.17	0.17
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD11	7	0.26	0.17	0.17
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	7	0.25	0.15	0.14
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	7	0.25	0.13	0.25
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD3	7	0.25	0.13	0.25
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	7	0.25	0.03	0.24
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	7	0.25	0.09	0.22
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	7	0.25	0.03	0.23
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	7	0.23	0.14	0.16
(2,262)	1:60:B:LYS:HD2	1:60:B:LYS:HA	7	0.23	0.14	0.16
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD11	7	0.21	0.04	0.22
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD13	7	0.21	0.04	0.22
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD12	7	0.21	0.04	0.22
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	7	0.2	0.07	0.21
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD12	7	0.19	0.06	0.19
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD11	7	0.19	0.06	0.19
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD13	7	0.19	0.06	0.19
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	7	0.19	0.05	0.2
(2,719)	1:56:B:GLU:HA	1:56:B:GLU:HG2	7	0.19	0.05	0.2
(2,720)	1:22:B:LEU:HG	1:22:B:LEU:HA	7	0.18	0.04	0.18
(2,720)	1:25:B:LEU:HB2	1:22:B:LEU:HA	7	0.18	0.04	0.18
(2,720)	1:85:B:LEU:HG	1:85:B:LEU:HA	7	0.18	0.04	0.18
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	7	0.18	0.07	0.15
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	7	0.17	0.04	0.17
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	7	0.15	0.05	0.11
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	7	0.14	0.02	0.13
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	7	0.12	0.02	0.12
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	7	0.12	0.02	0.12
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	6	0.96	0.36	1.0
(2,549)	1:17:B:SER:HB2	1:9:B:MET:HE1	6	0.94	0.23	0.84
(2,549)	1:83:B:ARG:HG2	1:84:B:SER:HB2	6	0.94	0.23	0.84
(2,651)	1:24:B:ASP:HB3	1:21:B:LEU:HD21	6	0.92	0.24	0.94
(2,651)	1:36:B:LEU:HD11	1:35:B:ASP:HB3	6	0.92	0.24	0.94
(2,651)	1:24:B:ASP:HB3	1:21:B:LEU:HD22	6	0.92	0.24	0.94
(2,651)	1:33:B:ASP:HB3	1:36:B:LEU:HD11	6	0.92	0.24	0.94
(2,651)	1:33:B:ASP:HB3	1:36:B:LEU:HD12	6	0.92	0.24	0.94
(2,988)	1:59:B:LYS:HB2	1:55:B:PRO:HB3	6	0.85	0.32	0.93
(2,988)	1:60:B:LYS:HB2	1:64:B:GLU:HG2	6	0.85	0.32	0.93
(2,988)	1:-1:B:LYS:HB2	1:0:B:MET:HG3	6	0.85	0.32	0.93
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	6	0.83	0.28	0.92
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD13	6	0.73	0.33	0.76
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD12	6	0.73	0.33	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD11	6	0.73	0.33	0.76
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	6	0.72	0.03	0.71
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD2	6	0.72	0.03	0.71
(2,902)	1:81:B:TRP:HB3	1:73:B:ILE:HD12	6	0.68	0.52	0.7
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE3	6	0.68	0.52	0.7
(2,902)	1:81:B:TRP:HB3	1:73:B:ILE:HD13	6	0.68	0.52	0.7
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE1	6	0.68	0.52	0.7
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE2	6	0.68	0.52	0.7
(2,1048)	1:31:B:ILE:HG12	1:30:B:PHE:HA	6	0.65	0.3	0.7
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	6	0.65	0.3	0.7
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	6	0.6	0.65	0.32
(2,967)	1:64:B:GLU:HG3	1:63:B:ASP:HB3	6	0.58	0.55	0.38
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE2	6	0.58	0.55	0.38
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE3	6	0.58	0.55	0.38
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE1	6	0.53	0.22	0.52
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE2	6	0.53	0.22	0.52
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE3	6	0.53	0.22	0.52
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	6	0.52	0.05	0.51
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	6	0.48	0.25	0.44
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	6	0.43	0.03	0.43
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD2	6	0.43	0.03	0.43
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	6	0.43	0.16	0.5
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	6	0.42	0.02	0.42
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	6	0.41	0.23	0.3
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD11	6	0.41	0.23	0.3
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	6	0.41	0.23	0.3
(2,1096)	1:39:B:ARG:HD2	1:98:B:LEU:HD12	6	0.41	0.23	0.3
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE2	6	0.41	0.17	0.4
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE3	6	0.41	0.17	0.4
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	6	0.4	0.19	0.44
(2,101)	1:74:B:ASN:HB2	1:75:B:SER:HA	6	0.4	0.19	0.44
(2,65)	1:72:B:LYS:HE2	1:72:B:LYS:HG3	6	0.39	0.23	0.32
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	6	0.39	0.23	0.32
(2,845)	1:100:B:PRO:HD3	1:43:B:ILE:HG13	6	0.39	0.1	0.38
(2,845)	1:100:B:PRO:HD3	1:101:B:LYS:HG3	6	0.39	0.1	0.38
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	6	0.38	0.09	0.36
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD23	6	0.33	0.08	0.33
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD21	6	0.33	0.08	0.33
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD22	6	0.33	0.08	0.33
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	6	0.31	0.01	0.32
(1,728)	1:26:B:ILE:HD12	1:86:B:GLY:HA3	6	0.3	0.08	0.34
(1,728)	1:26:B:ILE:HD13	1:86:B:GLY:HA3	6	0.3	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD12	6	0.3	0.13	0.3
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD13	6	0.3	0.13	0.3
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD11	6	0.3	0.13	0.3
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD12	6	0.29	0.07	0.28
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD11	6	0.29	0.07	0.28
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD13	6	0.29	0.07	0.28
(2,216)	1:8:B:GLU:HB3	1:7:B:ASN:HB3	6	0.28	0.1	0.26
(2,216)	1:8:B:GLU:HB2	1:74:B:ASN:HB2	6	0.28	0.1	0.26
(2,216)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	6	0.28	0.1	0.26
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD2	6	0.28	0.17	0.22
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD3	6	0.28	0.17	0.22
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	6	0.27	0.13	0.2
(2,8)	1:35:B:ASP:H	1:33:B:ASP:HB2	6	0.26	0.11	0.23
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD2	6	0.26	0.11	0.23
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD3	6	0.26	0.11	0.23
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	6	0.26	0.08	0.26
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	6	0.25	0.12	0.22
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	6	0.24	0.1	0.2
(2,35)	1:37:B:LYS:HE2	1:41:B:ASP:H	6	0.24	0.1	0.2
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD13	6	0.22	0.08	0.22
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD12	6	0.22	0.08	0.22
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG23	6	0.22	0.08	0.18
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG22	6	0.22	0.08	0.18
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG21	6	0.22	0.08	0.18
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	6	0.22	0.04	0.23
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	6	0.21	0.07	0.22
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB1	6	0.21	0.06	0.22
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB3	6	0.21	0.06	0.22
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB2	6	0.21	0.06	0.22
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	6	0.21	0.08	0.2
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	6	0.2	0.09	0.18
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD1	6	0.19	0.06	0.16
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD2	6	0.19	0.06	0.16
(2,153)	1:56:B:GLU:HG3	1:53:B:LEU:HA	6	0.18	0.09	0.15
(2,153)	1:76:B:GLU:HG2	1:77:B:THR:HA	6	0.18	0.09	0.15
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	6	0.18	0.05	0.18
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	6	0.17	0.08	0.14
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	6	0.16	0.03	0.18
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	6	0.16	0.05	0.15
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	6	0.15	0.03	0.14
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	6	0.14	0.02	0.14
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	6	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	5	1.02	0.24	1.1
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG22	5	0.87	0.02	0.88
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG23	5	0.87	0.02	0.88
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG21	5	0.87	0.02	0.88
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	5	0.87	0.11	0.92
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG21	5	0.78	0.1	0.75
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG23	5	0.78	0.1	0.75
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB2	5	0.72	0.18	0.79
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB3	5	0.72	0.18	0.79
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB1	5	0.72	0.18	0.79
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	5	0.71	0.22	0.81
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD13	5	0.59	0.05	0.6
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD11	5	0.59	0.05	0.6
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD12	5	0.59	0.05	0.6
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	5	0.59	0.06	0.61
(2,1506)	1:95:B:GLU:H	1:98:B:LEU:HD11	5	0.56	0.2	0.65
(2,1506)	1:16:B:ASN:H	1:15:B:LEU:HD22	5	0.56	0.2	0.65
(2,1506)	1:16:B:ASN:H	1:15:B:LEU:HD21	5	0.56	0.2	0.65
(2,1506)	1:95:B:GLU:H	1:96:B:LYS:HB2	5	0.56	0.2	0.65
(2,906)	1:99:B:ILE:HD11	1:99:B:ILE:HB	5	0.51	0.0	0.51
(2,906)	1:99:B:ILE:HD12	1:99:B:ILE:HB	5	0.51	0.0	0.51
(2,906)	1:99:B:ILE:HD13	1:99:B:ILE:HB	5	0.51	0.0	0.51
(2,1000)	1:53:B:LEU:H	1:51:B:VAL:HB	5	0.5	0.05	0.52
(2,1000)	1:30:B:PHE:H	1:28:B:LYS:HB3	5	0.5	0.05	0.52
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	5	0.49	0.06	0.51
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD12	5	0.47	0.14	0.53
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD11	5	0.47	0.14	0.53
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD13	5	0.47	0.14	0.53
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG21	5	0.45	0.17	0.45
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG22	5	0.45	0.17	0.45
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG23	5	0.45	0.17	0.45
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	5	0.43	0.06	0.45
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	5	0.41	0.0	0.41
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	5	0.41	0.03	0.39
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	5	0.41	0.11	0.46
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	5	0.4	0.04	0.41
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	5	0.38	0.07	0.41
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG11	5	0.37	0.17	0.3
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG12	5	0.37	0.17	0.3
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	5	0.37	0.02	0.36
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD13	5	0.37	0.05	0.38
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD11	5	0.37	0.05	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD12	5	0.37	0.05	0.38
(1,844)	1:54:B:ILE:HD13	1:89:B:ILE:HG23	5	0.35	0.11	0.35
(1,844)	1:54:B:ILE:HD11	1:89:B:ILE:HG23	5	0.35	0.11	0.35
(1,844)	1:54:B:ILE:HD12	1:89:B:ILE:HG22	5	0.35	0.11	0.35
(1,844)	1:54:B:ILE:HD12	1:89:B:ILE:HG21	5	0.35	0.11	0.35
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	5	0.35	0.18	0.35
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	5	0.32	0.1	0.37
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	5	0.32	0.04	0.31
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	5	0.3	0.03	0.28
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	5	0.29	0.12	0.3
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	5	0.29	0.09	0.3
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE2	5	0.29	0.17	0.23
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE1	5	0.29	0.17	0.23
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	5	0.29	0.09	0.32
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	5	0.28	0.02	0.27
(1,615)	1:43:B:ILE:HD13	1:98:B:LEU:HA	5	0.26	0.08	0.24
(1,615)	1:43:B:ILE:HD12	1:98:B:LEU:HA	5	0.26	0.08	0.24
(1,615)	1:43:B:ILE:HD11	1:98:B:LEU:HA	5	0.26	0.08	0.24
(2,1097)	1:98:B:LEU:HD22	1:39:B:ARG:HA	5	0.26	0.14	0.2
(2,1097)	1:98:B:LEU:HD21	1:39:B:ARG:HA	5	0.26	0.14	0.2
(2,1097)	1:98:B:LEU:HD23	1:39:B:ARG:HA	5	0.26	0.14	0.2
(2,1540)	1:96:B:LYS:H	1:96:B:LYS:HG2	5	0.26	0.07	0.26
(2,1540)	1:72:B:LYS:H	1:72:B:LYS:HG2	5	0.26	0.07	0.26
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE2	5	0.25	0.07	0.28
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE1	5	0.25	0.07	0.28
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE3	5	0.25	0.07	0.28
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD13	5	0.24	0.11	0.23
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD11	5	0.24	0.11	0.23
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD12	5	0.24	0.11	0.23
(2,768)	1:56:B:GLU:HG3	1:53:B:LEU:HA	5	0.24	0.07	0.27
(2,768)	1:64:B:GLU:HB3	1:65:B:LEU:HA	5	0.24	0.07	0.27
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD23	5	0.24	0.19	0.16
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD22	5	0.24	0.19	0.16
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD21	5	0.24	0.19	0.16
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	5	0.24	0.1	0.27
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	5	0.22	0.06	0.26
(2,1439)	1:60:B:LYS:H	1:59:B:LYS:HG3	5	0.22	0.06	0.23
(2,1439)	1:22:B:LEU:H	1:18:B:MET:HG3	5	0.22	0.06	0.23
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	5	0.21	0.06	0.2
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB3	5	0.2	0.01	0.2
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB2	5	0.2	0.01	0.2
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB1	5	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE1	5	0.2	0.02	0.2
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE3	5	0.2	0.02	0.2
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE2	5	0.2	0.02	0.2
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	5	0.18	0.03	0.19
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD11	5	0.18	0.04	0.17
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD12	5	0.18	0.04	0.17
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	5	0.17	0.03	0.17
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	5	0.17	0.03	0.16
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD12	5	0.16	0.04	0.17
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD13	5	0.16	0.04	0.17
(2,1532)	1:98:B:LEU:H	1:45:B:MET:HE1	5	0.16	0.04	0.17
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD11	5	0.16	0.04	0.17
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	5	0.14	0.01	0.15
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	5	0.13	0.02	0.14
(2,12)	1:83:B:ARG:HD2	1:83:B:ARG:HG2	5	0.12	0.01	0.11
(2,12)	1:83:B:ARG:HD3	1:83:B:ARG:HG2	5	0.12	0.01	0.11
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	5	0.11	0.01	0.11
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	4	1.6	0.04	1.6
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD21	4	1.6	0.04	1.6
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD23	4	1.6	0.04	1.6
(2,27)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	4	1.12	0.54	1.42
(2,27)	1:24:B:ASP:HB3	1:25:B:LEU:HD13	4	1.12	0.54	1.42
(2,27)	1:33:B:ASP:HB3	1:36:B:LEU:HD23	4	1.12	0.54	1.42
(2,955)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	4	0.9	0.11	0.9
(2,955)	1:8:B:GLU:HB3	1:7:B:ASN:HB3	4	0.9	0.11	0.9
(2,1436)	1:60:B:LYS:H	1:63:B:ASP:HB3	4	0.85	0.67	0.74
(2,1436)	1:60:B:LYS:H	1:96:B:LYS:HE3	4	0.85	0.67	0.74
(1,677)	1:5:B:ASN:HA	1:6:B:PRO:HD2	4	0.6	0.12	0.56
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE2	4	0.58	0.02	0.57
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE3	4	0.58	0.02	0.57
(2,169)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	4	0.56	0.33	0.48
(2,1018)	1:22:B:LEU:H	1:18:B:MET:HG3	4	0.55	0.67	0.19
(2,178)	1:49:B:GLN:HG3	1:52:B:THR:HG22	4	0.48	0.23	0.47
(2,178)	1:62:B:GLN:HG3	1:19:B:THR:HG21	4	0.48	0.23	0.47
(2,178)	1:49:B:GLN:HG3	1:52:B:THR:HG23	4	0.48	0.23	0.47
(2,186)	1:97:B:HIS:H	1:97:B:HIS:HB3	4	0.42	0.01	0.42
(2,186)	1:98:B:LEU:H	1:97:B:HIS:HB3	4	0.42	0.01	0.42
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD13	4	0.42	0.09	0.38
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD11	4	0.42	0.09	0.38
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD12	4	0.42	0.09	0.38
(1,690)	1:26:B:ILE:HD11	1:30:B:PHE:HE2	4	0.4	0.2	0.44
(1,690)	1:26:B:ILE:HD11	1:30:B:PHE:HE1	4	0.4	0.2	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,690)	1:26:B:ILE:HD12	1:30:B:PHE:HE2	4	0.4	0.2	0.44
(2,1580)	1:24:B:ASP:H	1:25:B:LEU:HB2	4	0.4	0.13	0.44
(2,1456)	1:93:B:PHE:H	1:54:B:ILE:HG23	4	0.39	0.12	0.36
(2,1456)	1:93:B:PHE:H	1:54:B:ILE:HG22	4	0.39	0.12	0.36
(2,1456)	1:93:B:PHE:H	1:96:B:LYS:HB2	4	0.39	0.12	0.36
(2,1478)	1:27:B:CYS:H	1:54:B:ILE:HG22	4	0.38	0.19	0.36
(2,528)	1:22:B:LEU:HD23	1:86:B:GLY:HA3	4	0.37	0.22	0.32
(2,528)	1:22:B:LEU:HD22	1:86:B:GLY:HA3	4	0.37	0.22	0.32
(2,909)	1:99:B:ILE:HD13	1:95:B:GLU:HG2	4	0.36	0.17	0.38
(2,909)	1:99:B:ILE:HD12	1:95:B:GLU:HG2	4	0.36	0.17	0.38
(2,909)	1:99:B:ILE:HD11	1:95:B:GLU:HG2	4	0.36	0.17	0.38
(2,934)	1:24:B:ASP:HB3	1:25:B:LEU:HB3	4	0.36	0.11	0.34
(2,934)	1:24:B:ASP:HB3	1:21:B:LEU:HB3	4	0.36	0.11	0.34
(2,1137)	1:24:B:ASP:HA	1:28:B:LYS:HG3	4	0.36	0.34	0.2
(2,1137)	1:24:B:ASP:HA	1:25:B:LEU:HG	4	0.36	0.34	0.2
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG23	4	0.34	0.21	0.26
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG22	4	0.34	0.21	0.26
(2,1381)	1:30:B:PHE:H	1:26:B:ILE:HB	4	0.33	0.06	0.34
(2,1381)	1:30:B:PHE:H	1:28:B:LYS:HG3	4	0.33	0.06	0.34
(2,38)	1:60:B:LYS:HE2	1:60:B:LYS:HB2	4	0.32	0.2	0.26
(2,38)	1:-1:B:LYS:HE3	1:-1:B:LYS:HB2	4	0.32	0.2	0.26
(2,925)	1:83:B:ARG:H	1:83:B:ARG:HD2	4	0.32	0.15	0.32
(2,91)	1:90:B:GLY:H	1:93:B:PHE:HB3	4	0.29	0.16	0.24
(2,737)	1:51:B:VAL:H	1:49:B:GLN:HA	4	0.28	0.07	0.29
(2,712)	1:51:B:VAL:HG13	1:47:B:TYR:HE1	4	0.27	0.18	0.18
(2,712)	1:51:B:VAL:HG12	1:47:B:TYR:HE1	4	0.27	0.18	0.18
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG22	4	0.26	0.11	0.24
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG23	4	0.26	0.11	0.24
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG21	4	0.26	0.11	0.24
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE2	4	0.25	0.07	0.26
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE1	4	0.25	0.07	0.26
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD13	4	0.23	0.1	0.2
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD11	4	0.23	0.1	0.2
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB1	4	0.21	0.11	0.18
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB2	4	0.21	0.11	0.18
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB3	4	0.21	0.11	0.18
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD12	4	0.21	0.08	0.2
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD11	4	0.21	0.08	0.2
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD13	4	0.21	0.08	0.2
(2,1054)	1:54:B:ILE:HA	1:26:B:ILE:HG13	4	0.21	0.08	0.22
(2,1054)	1:26:B:ILE:HG13	1:90:B:GLY:HA2	4	0.21	0.08	0.22
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD22	4	0.21	0.09	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD23	4	0.21	0.09	0.18
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD21	4	0.21	0.09	0.18
(2,1039)	1:49:B:GLN:HB2	1:46:B:THR:HG23	4	0.2	0.02	0.2
(2,1039)	1:49:B:GLN:HB3	1:46:B:THR:HG23	4	0.2	0.02	0.2
(2,1039)	1:49:B:GLN:HB2	1:46:B:THR:HG21	4	0.2	0.02	0.2
(1,1318)	1:43:B:ILE:H	1:39:B:ARG:HG2	4	0.2	0.06	0.19
(2,1440)	1:60:B:LYS:H	1:63:B:ASP:HB2	4	0.2	0.06	0.16
(2,1440)	1:22:B:LEU:H	1:24:B:ASP:HB2	4	0.2	0.06	0.16
(2,17)	1:92:B:ASP:HB3	1:57:B:SER:HA	4	0.2	0.05	0.2
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB1	4	0.19	0.05	0.2
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB2	4	0.19	0.05	0.2
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD11	4	0.18	0.08	0.16
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD12	4	0.18	0.08	0.16
(2,769)	1:53:B:LEU:HB2	1:53:B:LEU:HA	4	0.18	0.07	0.18
(2,769)	1:65:B:LEU:HB2	1:65:B:LEU:HA	4	0.18	0.07	0.18
(2,769)	1:21:B:LEU:HB2	1:18:B:MET:HA	4	0.18	0.07	0.18
(1,824)	1:99:B:ILE:HG21	1:101:B:LYS:HA	4	0.17	0.05	0.18
(1,824)	1:99:B:ILE:HG23	1:101:B:LYS:HA	4	0.17	0.05	0.18
(1,824)	1:99:B:ILE:HG22	1:101:B:LYS:HA	4	0.17	0.05	0.18
(2,785)	1:54:B:ILE:HG21	1:23:B:PRO:HD3	4	0.16	0.04	0.16
(2,785)	1:54:B:ILE:HG22	1:23:B:PRO:HD3	4	0.16	0.04	0.16
(2,785)	1:54:B:ILE:HG23	1:23:B:PRO:HD3	4	0.16	0.04	0.16
(2,1124)	1:51:B:VAL:HG13	1:23:B:PRO:HG2	4	0.16	0.05	0.13
(2,1124)	1:51:B:VAL:HG11	1:23:B:PRO:HG2	4	0.16	0.05	0.13
(2,1124)	1:51:B:VAL:HG12	1:23:B:PRO:HG2	4	0.16	0.05	0.13
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB2	4	0.15	0.04	0.15
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB3	4	0.15	0.04	0.15
(1,187)	1:97:B:HIS:H	1:96:B:LYS:HB3	4	0.15	0.02	0.14
(1,590)	1:78:B:ALA:HB2	1:73:B:ILE:HG23	4	0.14	0.03	0.14
(1,590)	1:78:B:ALA:HB1	1:73:B:ILE:HG23	4	0.14	0.03	0.14
(1,590)	1:78:B:ALA:HB2	1:73:B:ILE:HG22	4	0.14	0.03	0.14
(1,631)	1:43:B:ILE:HD11	1:100:B:PRO:HD3	4	0.14	0.03	0.13
(1,631)	1:43:B:ILE:HD12	1:100:B:PRO:HD3	4	0.14	0.03	0.13
(1,631)	1:43:B:ILE:HD13	1:100:B:PRO:HD3	4	0.14	0.03	0.13
(2,1031)	1:51:B:VAL:HA	1:23:B:PRO:HA	4	0.14	0.0	0.14
(2,614)	1:77:B:THR:HA	1:77:B:THR:HG22	4	0.14	0.01	0.14
(2,614)	1:77:B:THR:HA	1:77:B:THR:HG23	4	0.14	0.01	0.14
(2,614)	1:77:B:THR:HB	1:77:B:THR:HG23	4	0.14	0.01	0.14
(2,709)	1:51:B:VAL:HG22	1:52:B:THR:HA	4	0.14	0.02	0.12
(2,709)	1:51:B:VAL:HG23	1:52:B:THR:HA	4	0.14	0.02	0.12
(1,653)	1:31:B:ILE:HD13	1:47:B:TYR:HA	4	0.13	0.02	0.12
(2,1453)	1:93:B:PHE:H	1:91:B:LYS:HB2	4	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,406)	1:53:B:LEU:HG	1:53:B:LEU:HA	4	0.12	0.02	0.12
(2,214)	1:28:B:LYS:H	1:28:B:LYS:HB3	4	0.12	0.0	0.12
(1,1130)	1:39:B:ARG:H	1:38:B:LYS:HG2	4	0.12	0.01	0.12
(2,75)	1:36:B:LEU:HB3	1:37:B:LYS:HA	4	0.12	0.01	0.12
(1,703)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	3	1.05	1.09	0.34
(1,703)	1:85:B:LEU:HD12	1:82:B:GLY:HA3	3	1.05	1.09	0.34
(2,932)	1:44:B:LYS:HE2	1:44:B:LYS:HB2	3	0.73	0.17	0.85
(2,932)	1:60:B:LYS:HE3	1:60:B:LYS:HB2	3	0.73	0.17	0.85
(2,1020)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	3	0.59	0.13	0.65
(2,1361)	1:92:B:ASP:H	1:91:B:LYS:HE3	3	0.57	0.27	0.59
(2,1361)	1:92:B:ASP:H	1:60:B:LYS:HE3	3	0.57	0.27	0.59
(2,29)	1:25:B:LEU:HB2	1:22:B:LEU:HA	3	0.54	0.27	0.64
(2,29)	1:65:B:LEU:HB3	1:68:B:SER:HB2	3	0.54	0.27	0.64
(2,1175)	1:45:B:MET:HE2	1:40:B:PHE:HD2	3	0.54	0.24	0.37
(2,1175)	1:45:B:MET:HE3	1:40:B:PHE:HD1	3	0.54	0.24	0.37
(2,1175)	1:73:B:ILE:HG13	1:81:B:TRP:HD1	3	0.54	0.24	0.37
(2,939)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	3	0.53	0.38	0.44
(2,939)	1:34:B:PRO:HG2	1:35:B:ASP:HB2	3	0.53	0.38	0.44
(2,894)	1:14:B:TRP:HB3	1:69:B:MET:HE1	3	0.48	0.09	0.42
(2,634)	1:98:B:LEU:HD11	1:30:B:PHE:HE1	3	0.43	0.13	0.49
(2,634)	1:98:B:LEU:HD13	1:93:B:PHE:HE1	3	0.43	0.13	0.49
(2,634)	1:98:B:LEU:HD12	1:93:B:PHE:HE1	3	0.43	0.13	0.49
(2,187)	1:97:B:HIS:HB3	1:98:B:LEU:HG	3	0.43	0.09	0.43
(2,187)	1:97:B:HIS:HB3	1:43:B:ILE:HG13	3	0.43	0.09	0.43
(2,929)	1:-1:B:LYS:HE2	1:-1:B:LYS:HA	3	0.39	0.19	0.32
(2,929)	1:-1:B:LYS:HE3	1:-1:B:LYS:HA	3	0.39	0.19	0.32
(2,929)	1:61:B:CYS:HB2	1:57:B:SER:HB3	3	0.39	0.19	0.32
(1,866)	1:101:B:LYS:H	1:101:B:LYS:HG3	3	0.38	0.02	0.37
(1,455)	1:85:B:LEU:HD22	1:85:B:LEU:H	3	0.37	0.27	0.25
(1,455)	1:85:B:LEU:HD21	1:85:B:LEU:H	3	0.37	0.27	0.25
(2,181)	1:96:B:LYS:HE2	1:96:B:LYS:HB3	3	0.34	0.0	0.34
(2,1028)	1:38:B:LYS:HD3	1:39:B:ARG:H	3	0.34	0.12	0.31
(2,1028)	1:38:B:LYS:HD2	1:39:B:ARG:H	3	0.34	0.12	0.31
(2,1028)	1:43:B:ILE:H	1:44:B:LYS:HD2	3	0.34	0.12	0.31
(2,232)	1:28:B:LYS:HE3	1:28:B:LYS:HB2	3	0.33	0.07	0.37
(2,303)	1:61:B:CYS:H	1:60:B:LYS:HD3	3	0.33	0.15	0.39
(2,303)	1:61:B:CYS:H	1:60:B:LYS:HD2	3	0.33	0.15	0.39
(2,680)	1:28:B:LYS:HG2	1:28:B:LYS:HA	3	0.31	0.03	0.3
(1,52)	1:11:B:LYS:HE2	1:69:B:MET:HB3	3	0.28	0.06	0.29
(2,1088)	1:60:B:LYS:HG2	1:57:B:SER:HA	3	0.28	0.12	0.29
(2,1088)	1:-1:B:LYS:HG2	1:-2:B:ASP:HA	3	0.28	0.12	0.29
(1,1137)	1:60:B:LYS:H	1:60:B:LYS:HE3	3	0.27	0.03	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1072)	1:28:B:LYS:HG3	1:27:B:CYS:HB3	3	0.27	0.0	0.27
(2,1072)	1:28:B:LYS:HG3	1:32:B:GLN:HG3	3	0.27	0.0	0.27
(2,158)	1:25:B:LEU:H	1:26:B:ILE:HB	3	0.27	0.12	0.33
(2,1098)	1:98:B:LEU:HD22	1:39:B:ARG:HA	3	0.27	0.11	0.31
(2,1098)	1:98:B:LEU:HD21	1:39:B:ARG:HA	3	0.27	0.11	0.31
(1,895)	1:33:B:ASP:H	1:33:B:ASP:HB3	3	0.26	0.02	0.25
(1,1006)	1:94:B:ALA:H	1:96:B:LYS:HB3	3	0.26	0.04	0.27
(2,1179)	1:31:B:ILE:HG13	1:27:B:CYS:HA	3	0.26	0.06	0.24
(2,537)	1:36:B:LEU:HD21	1:35:B:ASP:HB2	3	0.24	0.08	0.2
(2,537)	1:36:B:LEU:HD23	1:35:B:ASP:HB2	3	0.24	0.08	0.2
(2,537)	1:85:B:LEU:HD12	1:81:B:TRP:HB3	3	0.24	0.08	0.2
(1,656)	1:31:B:ILE:HD11	1:40:B:PHE:HE2	3	0.24	0.03	0.26
(1,656)	1:31:B:ILE:HD11	1:40:B:PHE:HE1	3	0.24	0.03	0.26
(1,656)	1:31:B:ILE:HD13	1:40:B:PHE:HE1	3	0.24	0.03	0.26
(2,330)	1:39:B:ARG:HB3	1:98:B:LEU:HD22	3	0.24	0.09	0.25
(2,330)	1:39:B:ARG:HB3	1:98:B:LEU:HD21	3	0.24	0.09	0.25
(2,1451)	1:93:B:PHE:H	1:98:B:LEU:HG	3	0.24	0.05	0.26
(2,1451)	1:93:B:PHE:H	1:26:B:ILE:HG13	3	0.24	0.05	0.26
(2,454)	1:62:B:GLN:HB3	1:63:B:ASP:HB2	3	0.22	0.03	0.22
(2,454)	1:61:B:CYS:HB3	1:65:B:LEU:HG	3	0.22	0.03	0.22
(1,1121)	1:44:B:LYS:H	1:98:B:LEU:HD22	3	0.22	0.12	0.15
(1,1121)	1:44:B:LYS:H	1:98:B:LEU:HD21	3	0.22	0.12	0.15
(2,696)	1:28:B:LYS:HG2	1:28:B:LYS:HA	3	0.22	0.02	0.21
(1,203)	1:97:B:HIS:HB2	1:93:B:PHE:HD1	3	0.21	0.07	0.23
(1,203)	1:97:B:HIS:HB2	1:93:B:PHE:HD2	3	0.21	0.07	0.23
(2,946)	1:41:B:ASP:HB3	1:42:B:GLU:HG2	3	0.2	0.06	0.16
(2,1605)	1:97:B:HIS:H	1:98:B:LEU:HD22	3	0.2	0.07	0.17
(2,1605)	1:97:B:HIS:H	1:98:B:LEU:HD23	3	0.2	0.07	0.17
(2,897)	1:69:B:MET:HE3	1:11:B:LYS:HE2	3	0.18	0.06	0.19
(2,897)	1:69:B:MET:HE2	1:11:B:LYS:HE2	3	0.18	0.06	0.19
(1,820)	1:81:B:TRP:H	1:80:B:THR:HG22	3	0.18	0.01	0.18
(1,820)	1:81:B:TRP:H	1:80:B:THR:HG23	3	0.18	0.01	0.18
(1,942)	1:87:B:GLU:H	1:65:B:LEU:HD12	3	0.18	0.05	0.17
(1,942)	1:87:B:GLU:H	1:65:B:LEU:HD13	3	0.18	0.05	0.17
(2,1240)	1:87:B:GLU:H	1:83:B:ARG:HB2	3	0.18	0.09	0.11
(2,494)	1:83:B:ARG:HG3	1:87:B:GLU:HG2	3	0.17	0.05	0.17
(1,650)	1:43:B:ILE:HG22	1:97:B:HIS:HB3	3	0.17	0.05	0.15
(1,650)	1:43:B:ILE:HG23	1:97:B:HIS:HB3	3	0.17	0.05	0.15
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD13	3	0.17	0.03	0.15
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD12	3	0.17	0.03	0.15
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD11	3	0.17	0.03	0.15
(1,831)	1:4:B:ALA:HB3	1:5:B:ASN:HA	3	0.17	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,831)	1:4:B:ALA:HB1	1:5:B:ASN:HA	3	0.17	0.02	0.17
(1,831)	1:4:B:ALA:HB2	1:5:B:ASN:HA	3	0.17	0.02	0.17
(2,1420)	1:41:B:ASP:H	1:39:B:ARG:HG3	3	0.16	0.04	0.18
(2,1420)	1:41:B:ASP:H	1:37:B:LYS:HB2	3	0.16	0.04	0.18
(2,471)	1:39:B:ARG:HG3	1:39:B:ARG:HA	3	0.16	0.02	0.16
(2,175)	1:46:B:THR:H	1:49:B:GLN:HG2	3	0.15	0.03	0.15
(2,373)	1:101:B:LYS:H	1:101:B:LYS:HD2	3	0.15	0.03	0.17
(2,373)	1:23:B:PRO:HG2	1:24:B:ASP:H	3	0.15	0.03	0.17
(1,400)	1:28:B:LYS:HG3	1:28:B:LYS:HA	3	0.14	0.02	0.15
(2,1270)	1:54:B:ILE:H	1:51:B:VAL:HG12	3	0.14	0.02	0.15
(2,1270)	1:54:B:ILE:H	1:51:B:VAL:HG13	3	0.14	0.02	0.15
(2,771)	1:18:B:MET:HG2	1:18:B:MET:HA	3	0.13	0.04	0.1
(2,1376)	1:30:B:PHE:H	1:26:B:ILE:HA	3	0.13	0.02	0.13
(2,1376)	1:30:B:PHE:H	1:31:B:ILE:HA	3	0.13	0.02	0.13
(1,825)	1:93:B:PHE:H	1:89:B:ILE:HG23	3	0.12	0.0	0.12
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG21	3	0.12	0.01	0.13
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG22	3	0.12	0.01	0.13
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG23	3	0.12	0.01	0.13
(1,325)	1:81:B:TRP:HB3	1:81:B:TRP:HD1	3	0.12	0.0	0.12
(1,846)	1:96:B:LYS:HB2	1:97:B:HIS:HA	3	0.11	0.01	0.11
(2,714)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	2	1.58	0.0	1.58
(1,405)	1:18:B:MET:HG2	1:85:B:LEU:HD11	2	1.56	1.44	1.56
(1,75)	1:27:B:CYS:HB2	1:50:B:CYS:HB2	2	1.38	0.0	1.38
(1,114)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	2	1.19	0.0	1.19
(1,975)	1:62:B:GLN:H	1:63:B:ASP:HB3	2	1.05	0.05	1.05
(2,1494)	1:25:B:LEU:H	1:25:B:LEU:HD12	2	0.96	0.06	0.96
(2,1494)	1:25:B:LEU:H	1:25:B:LEU:HD13	2	0.96	0.06	0.96
(2,261)	1:45:B:MET:HG3	1:53:B:LEU:HD13	2	0.9	0.6	0.9
(2,261)	1:45:B:MET:HG3	1:53:B:LEU:HD11	2	0.9	0.6	0.9
(2,30)	1:25:B:LEU:HB2	1:26:B:ILE:HA	2	0.88	0.03	0.88
(1,87)	1:63:B:ASP:H	1:63:B:ASP:HB3	2	0.85	0.03	0.85
(1,28)	1:26:B:ILE:H	1:25:B:LEU:HB2	2	0.66	0.02	0.66
(2,915)	1:26:B:ILE:HG23	1:27:B:CYS:HB2	2	0.64	0.03	0.64
(2,915)	1:26:B:ILE:HG21	1:27:B:CYS:HB2	2	0.64	0.03	0.64
(2,937)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	2	0.64	0.38	0.64
(1,111)	1:51:B:VAL:H	1:50:B:CYS:HB2	2	0.62	0.01	0.62
(2,961)	1:50:B:CYS:HB3	1:54:B:ILE:HG12	2	0.57	0.08	0.57
(2,984)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	2	0.57	0.2	0.57
(2,16)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	2	0.54	0.08	0.54
(2,16)	1:92:B:ASP:HB2	1:60:B:LYS:HD2	2	0.54	0.08	0.54
(2,525)	1:98:B:LEU:H	1:45:B:MET:HE3	2	0.53	0.33	0.53
(2,525)	1:97:B:HIS:H	1:45:B:MET:HE3	2	0.53	0.33	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1553)	1:96:B:LYS:H	1:96:B:LYS:HE3	2	0.44	0.04	0.44
(2,405)	1:31:B:ILE:HG13	1:30:B:PHE:HB3	2	0.44	0.02	0.44
(1,549)	1:25:B:LEU:HB3	1:25:B:LEU:HA	2	0.42	0.0	0.42
(2,1535)	1:72:B:LYS:H	1:72:B:LYS:HE3	2	0.41	0.03	0.41
(1,766)	1:99:B:ILE:HG21	1:101:B:LYS:HB3	2	0.34	0.06	0.34
(1,766)	1:99:B:ILE:HG23	1:101:B:LYS:HB3	2	0.34	0.06	0.34
(2,1320)	1:40:B:PHE:H	1:38:B:LYS:HB3	2	0.33	0.06	0.33
(2,950)	1:67:B:ALA:HB1	1:66:B:TYR:HB3	2	0.33	0.04	0.33
(2,950)	1:67:B:ALA:HB3	1:66:B:TYR:HB3	2	0.33	0.04	0.33
(2,912)	1:96:B:LYS:HB2	1:96:B:LYS:HE3	2	0.32	0.03	0.32
(2,1324)	1:40:B:PHE:H	1:98:B:LEU:HD12	2	0.3	0.08	0.3
(2,1324)	1:40:B:PHE:H	1:98:B:LEU:HD11	2	0.3	0.08	0.3
(1,464)	1:98:B:LEU:HD11	1:40:B:PHE:HD2	2	0.29	0.06	0.29
(1,464)	1:98:B:LEU:HD13	1:40:B:PHE:HD1	2	0.29	0.06	0.29
(2,36)	1:37:B:LYS:HE3	1:31:B:ILE:HA	2	0.29	0.18	0.29
(2,36)	1:61:B:CYS:HB2	1:58:B:THR:HA	2	0.29	0.18	0.29
(2,1489)	1:27:B:CYS:H	1:27:B:CYS:HB3	2	0.29	0.0	0.29
(2,1489)	1:35:B:ASP:H	1:35:B:ASP:HB3	2	0.29	0.0	0.29
(1,568)	1:89:B:ILE:HG23	1:57:B:SER:HB2	2	0.26	0.02	0.26
(1,568)	1:89:B:ILE:HG22	1:57:B:SER:HB2	2	0.26	0.02	0.26
(1,1072)	1:64:B:GLU:H	1:63:B:ASP:HB3	2	0.26	0.02	0.26
(2,103)	1:30:B:PHE:HB3	1:40:B:PHE:HD1	2	0.26	0.05	0.26
(2,103)	1:30:B:PHE:HB3	1:40:B:PHE:HD2	2	0.26	0.05	0.26
(2,41)	1:37:B:LYS:HE3	1:31:B:ILE:HG23	2	0.24	0.0	0.24
(2,41)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	2	0.24	0.0	0.24
(1,771)	1:43:B:ILE:H	1:45:B:MET:HB3	2	0.22	0.08	0.22
(2,1158)	1:31:B:ILE:HD13	1:27:B:CYS:HB3	2	0.22	0.08	0.22
(2,963)	1:101:B:LYS:H	1:99:B:ILE:HB	2	0.2	0.04	0.2
(2,1148)	1:20:B:PRO:HD3	1:16:B:ASN:HA	2	0.2	0.03	0.2
(2,365)	1:33:B:ASP:H	1:32:B:GLN:HB3	2	0.2	0.07	0.2
(2,919)	1:96:B:LYS:HG3	1:96:B:LYS:HA	2	0.2	0.03	0.2
(2,62)	1:21:B:LEU:HB2	1:20:B:PRO:HD2	2	0.2	0.01	0.2
(2,848)	1:39:B:ARG:HD2	1:100:B:PRO:HD2	2	0.18	0.08	0.18
(2,756)	1:-1:B:LYS:HD3	1:-1:B:LYS:HA	2	0.17	0.04	0.17
(1,589)	1:78:B:ALA:HB3	1:14:B:TRP:HD1	2	0.16	0.01	0.16
(1,589)	1:78:B:ALA:HB1	1:14:B:TRP:HD1	2	0.16	0.01	0.16
(2,168)	1:54:B:ILE:HB	1:51:B:VAL:HG12	2	0.16	0.03	0.16
(2,168)	1:54:B:ILE:HB	1:51:B:VAL:HG13	2	0.16	0.03	0.16
(2,593)	1:15:B:LEU:HD21	1:62:B:GLN:HA	2	0.16	0.06	0.16
(2,593)	1:73:B:ILE:HG12	1:73:B:ILE:HA	2	0.16	0.06	0.16
(2,910)	1:31:B:ILE:HD12	1:47:B:TYR:HD1	2	0.16	0.05	0.16
(2,910)	1:31:B:ILE:HD13	1:40:B:PHE:HE1	2	0.16	0.05	0.16

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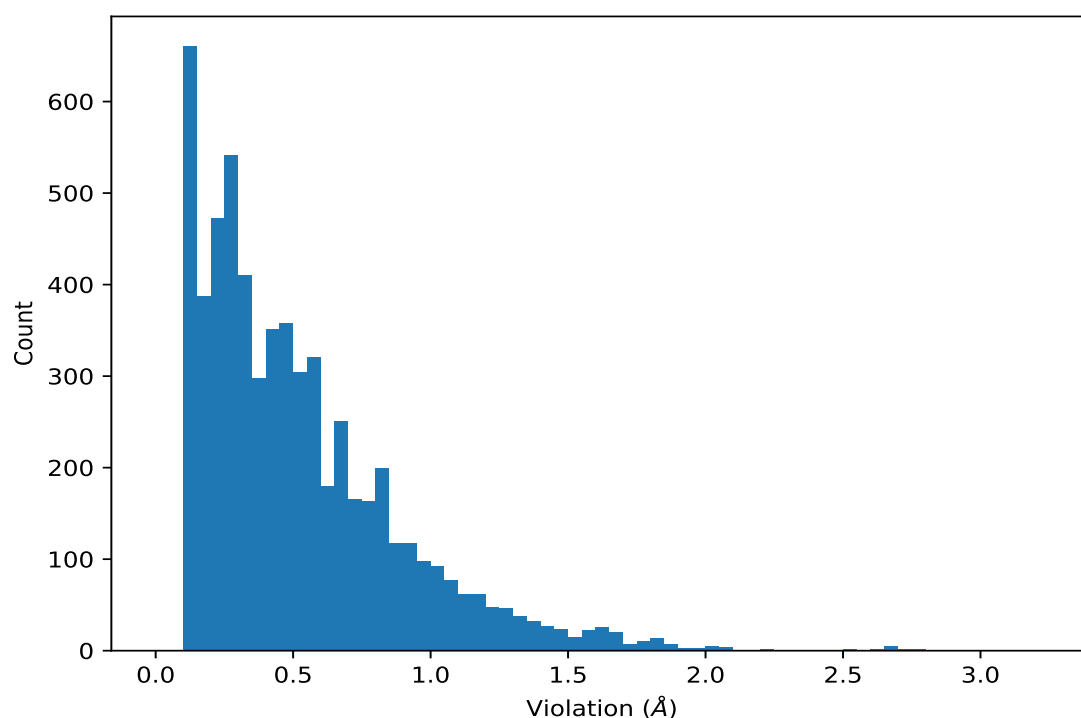
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1490)	1:35:B:ASP:H	1:36:B:LEU:HB2	2	0.16	0.02	0.16
(1,723)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	2	0.16	0.01	0.16
(2,571)	1:66:B:TYR:HA	1:68:B:SER:H	2	0.16	0.01	0.16
(2,833)	1:8:B:GLU:HB2	1:74:B:ASN:HA	2	0.15	0.02	0.15
(2,658)	1:27:B:CYS:HB2	1:27:B:CYS:HA	2	0.15	0.0	0.15
(2,1241)	1:87:B:GLU:H	1:89:B:ILE:HB	2	0.15	0.0	0.15
(2,1154)	1:99:B:ILE:HG21	1:101:B:LYS:HA	2	0.14	0.02	0.14
(2,1154)	1:99:B:ILE:HG22	1:101:B:LYS:HA	2	0.14	0.02	0.14
(2,558)	1:36:B:LEU:H	1:36:B:LEU:HD22	2	0.13	0.0	0.13
(2,558)	1:36:B:LEU:H	1:36:B:LEU:HD21	2	0.13	0.0	0.13
(2,1521)	1:56:B:GLU:H	1:55:B:PRO:HB3	2	0.13	0.01	0.13
(2,1574)	1:19:B:THR:H	1:20:B:PRO:HG2	2	0.12	0.02	0.12
(1,877)	1:74:B:ASN:H	1:73:B:ILE:HG21	2	0.12	0.0	0.12
(1,877)	1:74:B:ASN:H	1:73:B:ILE:HG22	2	0.12	0.0	0.12
(2,238)	1:9:B:MET:HG2	1:8:B:GLU:HA	2	0.12	0.0	0.12
(2,238)	1:9:B:MET:HG2	1:10:B:THR:HA	2	0.12	0.0	0.12
(2,49)	1:21:B:LEU:HB2	1:21:B:LEU:HA	2	0.11	0.0	0.11
(2,708)	1:24:B:ASP:H	1:51:B:VAL:HG11	2	0.11	0.0	0.11
(2,708)	1:24:B:ASP:H	1:51:B:VAL:HG12	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,798)	1:85:B:LEU:HD21	1:64:B:GLU:H	6	3.21
(1,458)	1:61:B:CYS:HB3	1:85:B:LEU:HD22	6	3.16
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	6	3.07
(1,405)	1:18:B:MET:HG2	1:85:B:LEU:HD11	6	3.01
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD23	4	2.91
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD22	2	2.78
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD23	9	2.77
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	10	2.72
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	3	2.7
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	4	2.68
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	9	2.68
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	1	2.67
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	8	2.66
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	8	2.66
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	10	2.61
(1,703)	1:85:B:LEU:HD12	1:82:B:GLY:HA3	6	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1143)	1:4:B:ALA:HB3	1:5:B:ASN:HB3	1	2.59
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	2	2.52
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	7	2.51
(1,701)	1:85:B:LEU:HB3	1:82:B:GLY:HA3	5	2.42
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD11	4	2.36
(2,682)	1:80:B:THR:HG23	1:83:B:ARG:HB3	9	2.26
(2,682)	1:80:B:THR:HG21	1:83:B:ARG:HB3	4	2.24
(2,885)	1:90:B:GLY:HA3	1:36:B:LEU:HD12	8	2.22
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	8	2.16
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD13	2	2.11
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	8	2.08
(2,564)	1:36:B:LEU:HD21	1:30:B:PHE:HA	6	2.07
(1,500)	1:36:B:LEU:HD11	1:36:B:LEU:HA	10	2.07
(2,682)	1:80:B:THR:HG21	1:83:B:ARG:HB3	3	2.06
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	7	2.05
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	2	2.03
(1,500)	1:36:B:LEU:HD13	1:36:B:LEU:HA	9	2.03
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD12	6	2.0
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	1	2.0
(2,1143)	1:78:B:ALA:HB2	1:74:B:ASN:HB2	7	1.98
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	4	1.98
(2,1143)	1:4:B:ALA:HB1	1:5:B:ASN:HB3	9	1.96
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	8	1.95
(2,1518)	1:65:B:LEU:H	1:85:B:LEU:HD21	6	1.91
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	8	1.91
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	1	1.89
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	5	1.88
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	7	1.88
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD13	3	1.88
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	6	1.87
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD23	7	1.86
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD11	5	1.85
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	4	1.84
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	3	1.83
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	5	1.83
(1,201)	1:97:B:HIS:HB2	1:53:B:LEU:HD13	4	1.83
(2,1004)	1:58:B:THR:HG23	1:20:B:PRO:HB2	4	1.82
(2,943)	1:13:B:ALA:HB2	1:12:B:ASP:HB2	5	1.82
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	8	1.82
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	2	1.81
(2,1436)	1:60:B:LYS:H	1:63:B:ASP:HB3	4	1.8
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	4	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	10	1.8
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	6	1.8
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	9	1.8
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	6	1.8
(2,1004)	1:58:B:THR:HG23	1:20:B:PRO:HB2	5	1.79
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	7	1.79
(2,236)	1:9:B:MET:HG3	1:72:B:LYS:HB3	1	1.79
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	2	1.79
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	10	1.78
(1,456)	1:85:B:LEU:HD21	1:85:B:LEU:HA	6	1.77
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	1	1.76
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	8	1.76
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	2	1.76
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	5	1.75
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	2	1.74
(2,1103)	1:36:B:LEU:HD13	1:35:B:ASP:HB2	8	1.74
(2,1004)	1:58:B:THR:HG21	1:20:B:PRO:HB2	3	1.74
(2,967)	1:64:B:GLU:HG3	1:63:B:ASP:HB3	7	1.73
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	1	1.73
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	10	1.73
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	10	1.71
(2,1018)	1:22:B:LEU:H	1:18:B:MET:HG3	8	1.7
(2,943)	1:71:B:ASP:HB2	1:72:B:LYS:HB2	3	1.7
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	6	1.7
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	5	1.7
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	5	1.69
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	3	1.69
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	7	1.69
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	9	1.69
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	2	1.68
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	4	1.68
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	3	1.68
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	4	1.68
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	1	1.67
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	3	1.67
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	7	1.67
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD11	8	1.67
(2,885)	1:90:B:GLY:HA3	1:36:B:LEU:HD13	9	1.66
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	5	1.66
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	8	1.66
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	4	1.66
(2,682)	1:80:B:THR:HG23	1:83:B:ARG:HB3	1	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	1	1.65
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	10	1.65
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	10	1.65
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	7	1.64
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	10	1.64
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	3	1.64
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD13	1	1.64
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD12	9	1.64
(2,1004)	1:58:B:THR:HG23	1:20:B:PRO:HB2	1	1.63
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD2	4	1.63
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	1	1.63
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	6	1.63
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	8	1.63
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	9	1.63
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD23	2	1.63
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD13	7	1.62
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG23	6	1.61
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG21	10	1.61
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	10	1.61
(2,155)	1:87:B:GLU:HG3	1:65:B:LEU:HD13	1	1.61
(2,117)	1:50:B:CYS:HB2	1:31:B:ILE:HD13	1	1.61
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	2	1.6
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	10	1.6
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD13	1	1.6
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	1	1.6
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG23	7	1.59
(2,1004)	1:58:B:THR:HG23	1:20:B:PRO:HB2	6	1.59
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	1	1.59
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	9	1.59
(2,256)	1:52:B:THR:HB	1:49:B:GLN:HG3	10	1.59
(2,129)	1:40:B:PHE:HB2	1:41:B:ASP:HB3	9	1.59
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD11	10	1.59
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	8	1.59
(2,1004)	1:58:B:THR:HG22	1:20:B:PRO:HB2	9	1.58
(2,714)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	3	1.58
(2,714)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	5	1.58
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	8	1.57
(1,427)	1:33:B:ASP:HB3	1:36:B:LEU:HD21	9	1.57
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG21	1	1.56
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	4	1.56
(2,256)	1:52:B:THR:HB	1:49:B:GLN:HG3	7	1.56
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD12	6	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	9	1.56
(2,943)	1:71:B:ASP:HB2	1:72:B:LYS:HB2	2	1.55
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	4	1.55
(2,256)	1:52:B:THR:HB	1:49:B:GLN:HG3	6	1.55
(1,784)	1:70:B:PRO:HG3	1:72:B:LYS:HA	2	1.55
(2,236)	1:9:B:MET:HG3	1:72:B:LYS:HB3	4	1.54
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD11	4	1.54
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG22	5	1.53
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	1	1.53
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	4	1.53
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG21	7	1.52
(1,539)	1:88:B:CYS:HB3	1:85:B:LEU:HA	1	1.52
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	3	1.51
(2,261)	1:45:B:MET:HG3	1:53:B:LEU:HD11	4	1.51
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	9	1.51
(2,236)	1:9:B:MET:HG3	1:18:B:MET:HB2	7	1.51
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD23	4	1.51
(2,682)	1:80:B:THR:HG22	1:83:B:ARG:HB3	2	1.5
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	3	1.5
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG22	9	1.5
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG22	2	1.49
(2,256)	1:52:B:THR:HB	1:49:B:GLN:HG3	2	1.49
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	6	1.49
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD22	10	1.49
(2,1103)	1:36:B:LEU:HD13	1:35:B:ASP:HB2	10	1.48
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	1	1.48
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	8	1.48
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD11	5	1.48
(2,1017)	1:64:B:GLU:HG2	1:60:B:LYS:HD2	3	1.47
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	10	1.47
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	10	1.47
(2,418)	1:69:B:MET:HG3	1:81:B:TRP:HB2	7	1.47
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	2	1.47
(2,27)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	10	1.47
(2,1382)	1:30:B:PHE:H	1:26:B:ILE:HG12	5	1.46
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	4	1.46
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD2	1	1.46
(2,827)	1:73:B:ILE:HG22	1:74:B:ASN:HB2	3	1.46
(2,825)	1:73:B:ILE:HG21	1:9:B:MET:HE3	1	1.46
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	8	1.46
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG23	10	1.46
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	5	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	8	1.46
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG23	3	1.45
(2,1106)	1:10:B:THR:HG23	1:71:B:ASP:HA	1	1.45
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG23	2	1.45
(2,27)	1:33:B:ASP:HB3	1:36:B:LEU:HD23	2	1.45
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD23	9	1.45
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	1	1.45
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	7	1.44
(2,561)	1:22:B:LEU:HD21	1:14:B:TRP:HZ2	6	1.44
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG21	3	1.44
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD13	2	1.44
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	4	1.44
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG21	4	1.43
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	3	1.43
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD11	10	1.43
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	5	1.43
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG23	1	1.42
(2,1122)	1:51:B:VAL:HG13	1:23:B:PRO:HD3	6	1.42
(2,1122)	1:51:B:VAL:HG13	1:23:B:PRO:HD3	10	1.42
(2,1044)	1:32:B:GLN:HB2	1:31:B:ILE:HG22	9	1.42
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	3	1.42
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	2	1.42
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	9	1.42
(2,1122)	1:51:B:VAL:HG11	1:23:B:PRO:HD3	3	1.41
(2,825)	1:73:B:ILE:HG21	1:18:B:MET:HG2	4	1.41
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD23	5	1.41
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	4	1.41
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	8	1.41
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG22	8	1.4
(2,1122)	1:51:B:VAL:HG11	1:23:B:PRO:HD3	5	1.4
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	8	1.4
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB1	3	1.4
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG22	5	1.39
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG22	3	1.39
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	2	1.39
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	4	1.39
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	6	1.39
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG22	1	1.39
(2,27)	1:33:B:ASP:HB3	1:36:B:LEU:HD22	8	1.39
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	9	1.38
(2,297)	1:42:B:GLU:HB2	1:43:B:ILE:HG21	6	1.38
(2,236)	1:9:B:MET:HG3	1:72:B:LYS:HB3	2	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	2	1.38
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG21	4	1.38
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	8	1.38
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB2	10	1.38
(1,75)	1:27:B:CYS:HB2	1:50:B:CYS:HB2	5	1.38
(2,1044)	1:95:B:GLU:HB2	1:96:B:LYS:HB2	7	1.37
(2,974)	1:95:B:GLU:HG3	1:99:B:ILE:HB	6	1.37
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD12	2	1.37
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD12	7	1.37
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	4	1.37
(1,75)	1:27:B:CYS:HB2	1:50:B:CYS:HB2	3	1.37
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	5	1.36
(2,1122)	1:51:B:VAL:HG13	1:23:B:PRO:HD3	1	1.35
(2,1044)	1:32:B:GLN:HB2	1:31:B:ILE:HG21	8	1.35
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD12	3	1.35
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	5	1.35
(1,702)	1:85:B:LEU:HG	1:82:B:GLY:HA3	1	1.35
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	2	1.35
(2,1382)	1:30:B:PHE:H	1:26:B:ILE:HG12	3	1.34
(2,651)	1:24:B:ASP:HB3	1:21:B:LEU:HD21	4	1.34
(2,549)	1:83:B:ARG:HG2	1:84:B:SER:HB2	9	1.34
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	7	1.34
(1,457)	1:85:B:LEU:HD22	1:62:B:GLN:HA	6	1.34
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	3	1.34
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB1	9	1.34
(2,1143)	1:4:B:ALA:HB1	1:5:B:ASN:HB3	5	1.33
(2,1122)	1:51:B:VAL:HG12	1:23:B:PRO:HD3	9	1.33
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD11	1	1.33
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	3	1.33
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG22	2	1.32
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	6	1.32
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD22	6	1.32
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	8	1.32
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	4	1.32
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	4	1.32
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	2	1.31
(2,1030)	1:54:B:ILE:HG12	1:27:B:CYS:HB3	10	1.31
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	4	1.31
(2,825)	1:73:B:ILE:HG22	1:18:B:MET:HG2	2	1.31
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD13	10	1.31
(2,144)	1:95:B:GLU:HG3	1:99:B:ILE:HB	5	1.31
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	10	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	9	1.31
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	3	1.31
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	9	1.31
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG21	10	1.3
(2,1164)	1:54:B:ILE:HD13	1:55:B:PRO:HD2	6	1.3
(2,1044)	1:95:B:GLU:HB2	1:96:B:LYS:HB2	4	1.3
(2,988)	1:59:B:LYS:HB2	1:55:B:PRO:HB3	4	1.3
(2,825)	1:73:B:ILE:HG22	1:9:B:MET:HE2	3	1.3
(2,824)	1:73:B:ILE:HG21	1:70:B:PRO:HG3	5	1.3
(2,627)	1:15:B:LEU:HD11	1:14:B:TRP:H	3	1.3
(2,564)	1:85:B:LEU:HD13	1:82:B:GLY:HA3	9	1.3
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	10	1.3
(2,127)	1:50:B:CYS:HB2	1:31:B:ILE:HD11	8	1.3
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	4	1.3
(2,1164)	1:54:B:ILE:HD13	1:55:B:PRO:HD2	4	1.29
(2,1164)	1:54:B:ILE:HD11	1:55:B:PRO:HD2	9	1.29
(2,824)	1:73:B:ILE:HG23	1:70:B:PRO:HG3	2	1.29
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD11	7	1.29
(2,256)	1:19:B:THR:HB	1:20:B:PRO:HB2	8	1.29
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	3	1.29
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	6	1.29
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	8	1.29
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	10	1.29
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	10	1.29
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD11	2	1.29
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB1	1	1.29
(2,1608)	1:52:B:THR:H	1:54:B:ILE:HG22	9	1.28
(2,220)	1:18:B:MET:HE3	1:18:B:MET:HB3	8	1.28
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG23	3	1.28
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	8	1.28
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	2	1.28
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	5	1.28
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	5	1.28
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	4	1.28
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	4	1.28
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	7	1.28
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	5	1.28
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	8	1.28
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG22	1	1.27
(2,824)	1:73:B:ILE:HG22	1:70:B:PRO:HG3	8	1.27
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	7	1.27
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	4	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB1	8	1.27
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG23	4	1.26
(2,1203)	1:89:B:ILE:H	1:60:B:LYS:HD3	5	1.26
(2,824)	1:73:B:ILE:HG23	1:70:B:PRO:HG3	7	1.26
(2,286)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	9	1.26
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	1	1.26
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	7	1.26
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	1	1.25
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	6	1.25
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG21	5	1.25
(2,1143)	1:4:B:ALA:HB3	1:5:B:ASN:HB3	6	1.25
(2,824)	1:73:B:ILE:HG22	1:70:B:PRO:HG3	4	1.25
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	9	1.25
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	9	1.25
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	2	1.25
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	9	1.25
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	2	1.25
(1,97)	1:66:B:TYR:HB2	1:67:B:ALA:HB3	6	1.25
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	4	1.24
(2,1369)	1:58:B:THR:H	1:59:B:LYS:HD3	8	1.24
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG23	8	1.24
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB3	7	1.24
(2,1164)	1:54:B:ILE:HD11	1:55:B:PRO:HD2	8	1.24
(2,827)	1:73:B:ILE:HG21	1:74:B:ASN:HB2	1	1.24
(2,824)	1:73:B:ILE:HG21	1:70:B:PRO:HG3	3	1.24
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD11	8	1.24
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	2	1.24
(1,978)	1:62:B:GLN:H	1:85:B:LEU:HD22	6	1.24
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	1	1.24
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	7	1.24
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	1	1.24
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	7	1.24
(2,827)	1:73:B:ILE:HG23	1:74:B:ASN:HB2	10	1.23
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	10	1.23
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	3	1.23
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	9	1.22
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG21	2	1.22
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG22	3	1.22
(2,1143)	1:4:B:ALA:HB3	1:5:B:ASN:HB3	8	1.22
(2,1106)	1:10:B:THR:HG21	1:71:B:ASP:HA	4	1.22
(2,902)	1:81:B:TRP:HB3	1:73:B:ILE:HD12	2	1.22
(2,902)	1:81:B:TRP:HB3	1:73:B:ILE:HD13	7	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	3	1.22
(2,825)	1:73:B:ILE:HG23	1:9:B:MET:HE1	10	1.22
(2,824)	1:73:B:ILE:HG22	1:70:B:PRO:HG3	6	1.22
(2,824)	1:73:B:ILE:HG22	1:70:B:PRO:HG3	10	1.22
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	1	1.22
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	3	1.22
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	1	1.22
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	5	1.22
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	2	1.22
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	5	1.21
(2,1164)	1:54:B:ILE:HD12	1:55:B:PRO:HD2	7	1.21
(2,1106)	1:10:B:THR:HG23	1:71:B:ASP:HA	5	1.21
(2,974)	1:95:B:GLU:HG3	1:99:B:ILE:HB	8	1.21
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	8	1.21
(2,667)	1:98:B:LEU:HD13	1:39:B:ARG:H	4	1.21
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	10	1.21
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	10	1.21
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD21	1	1.21
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	10	1.21
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	6	1.21
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	9	1.21
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	10	1.21
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD11	3	1.21
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	5	1.21
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG23	6	1.2
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG22	7	1.2
(2,1258)	1:53:B:LEU:H	1:54:B:ILE:HG23	9	1.2
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	9	1.2
(2,824)	1:73:B:ILE:HG23	1:70:B:PRO:HG3	9	1.2
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	8	1.2
(1,498)	1:47:B:TYR:HB2	1:48:B:GLU:HA	4	1.2
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	2	1.2
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	4	1.2
(2,1304)	1:15:B:LEU:H	1:85:B:LEU:HD23	7	1.19
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG21	5	1.19
(2,1164)	1:54:B:ILE:HD12	1:55:B:PRO:HD2	2	1.19
(2,1164)	1:54:B:ILE:HD12	1:55:B:PRO:HD2	3	1.19
(2,1164)	1:54:B:ILE:HD12	1:55:B:PRO:HD2	5	1.19
(2,1143)	1:4:B:ALA:HB3	1:5:B:ASN:HB3	3	1.19
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	4	1.19
(2,974)	1:95:B:GLU:HG3	1:99:B:ILE:HB	9	1.19
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD11	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD11	2	1.19
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD23	3	1.19
(2,127)	1:50:B:CYS:HB2	1:45:B:MET:HE2	5	1.19
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	8	1.19
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	1	1.19
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	6	1.19
(1,114)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	3	1.19
(1,114)	1:50:B:CYS:HB2	1:51:B:VAL:HG13	5	1.19
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	8	1.18
(2,902)	1:81:B:TRP:HB3	1:73:B:ILE:HD12	1	1.18
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	1	1.18
(2,827)	1:73:B:ILE:HG23	1:74:B:ASN:HB2	8	1.18
(2,824)	1:73:B:ILE:HG23	1:70:B:PRO:HG3	1	1.18
(2,667)	1:98:B:LEU:HD11	1:39:B:ARG:H	5	1.18
(2,667)	1:99:B:ILE:H	1:98:B:LEU:HD13	6	1.18
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	3	1.18
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	2	1.18
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	4	1.18
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD22	4	1.18
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	9	1.18
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	5	1.18
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	6	1.18
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	7	1.18
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	10	1.17
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	7	1.17
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	3	1.17
(2,1436)	1:60:B:LYS:H	1:96:B:LYS:HE3	5	1.16
(2,1382)	1:30:B:PHE:H	1:28:B:LYS:HD2	6	1.16
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	7	1.16
(2,1144)	1:17:B:SER:HB2	1:13:B:ALA:HB3	5	1.16
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG22	2	1.16
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	9	1.16
(2,948)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	5	1.16
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD21	2	1.16
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD22	3	1.16
(2,638)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	6	1.16
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	3	1.16
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	8	1.16
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG23	4	1.16
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	8	1.16
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG21	6	1.16
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	10	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	3	1.16
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	2	1.16
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	6	1.15
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	7	1.15
(2,974)	1:55:B:PRO:HB2	1:56:B:GLU:HG3	7	1.15
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB2	8	1.15
(2,549)	1:83:B:ARG:HG2	1:84:B:SER:HB2	3	1.15
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	5	1.15
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	1	1.15
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD11	9	1.15
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	8	1.15
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	7	1.15
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD11	8	1.15
(2,1164)	1:54:B:ILE:HD13	1:55:B:PRO:HD2	1	1.14
(2,827)	1:73:B:ILE:HG21	1:74:B:ASN:HB2	9	1.14
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	10	1.14
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	5	1.14
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	4	1.14
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	7	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	1	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	2	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD22	9	1.14
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD21	10	1.14
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	10	1.14
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	1	1.14
(2,1164)	1:54:B:ILE:HD11	1:55:B:PRO:HD2	10	1.13
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	4	1.13
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	6	1.13
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	7	1.13
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	7	1.13
(1,569)	1:89:B:ILE:HG21	1:90:B:GLY:HA3	6	1.13
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	3	1.13
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	8	1.13
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG21	10	1.12
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB1	10	1.12
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	7	1.12
(2,974)	1:95:B:GLU:HG3	1:99:B:ILE:HB	5	1.12
(2,827)	1:73:B:ILE:HG23	1:74:B:ASN:HB2	4	1.12
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	5	1.12
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD22	7	1.12
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD13	6	1.12
(1,119)	1:47:B:TYR:HB3	1:31:B:ILE:HD11	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1144)	1:17:B:SER:HB2	1:13:B:ALA:HB1	9	1.11
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	2	1.11
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	3	1.11
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	8	1.11
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	2	1.11
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	6	1.11
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	5	1.11
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	2	1.11
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	8	1.11
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	9	1.11
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	3	1.11
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	8	1.1
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	4	1.1
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	10	1.1
(2,1106)	1:10:B:THR:HG23	1:71:B:ASP:HA	3	1.1
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD22	10	1.1
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	1	1.1
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD21	1	1.1
(1,975)	1:62:B:GLN:H	1:63:B:ASP:HB3	4	1.1
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	6	1.1
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	4	1.1
(1,569)	1:89:B:ILE:HG21	1:90:B:GLY:HA3	8	1.1
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG23	5	1.09
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	5	1.09
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	4	1.09
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	4	1.09
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	2	1.09
(2,1165)	1:54:B:ILE:HD12	1:50:B:CYS:HB2	6	1.09
(2,1116)	1:19:B:THR:HG23	1:62:B:GLN:HA	5	1.09
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE3	5	1.09
(2,628)	1:65:B:LEU:HD23	1:68:B:SER:HB3	3	1.09
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	9	1.09
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	3	1.09
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	7	1.09
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	6	1.09
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	5	1.08
(2,1168)	1:54:B:ILE:HD12	1:58:B:THR:HG22	8	1.08
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG22	2	1.08
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD12	2	1.08
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	7	1.08
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	9	1.08
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	4	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	8	1.08
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	10	1.08
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	7	1.08
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	7	1.08
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	7	1.07
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB2	4	1.07
(2,1366)	1:11:B:LYS:H	1:72:B:LYS:HB2	6	1.07
(2,1168)	1:54:B:ILE:HD12	1:58:B:THR:HG23	9	1.07
(2,1048)	1:31:B:ILE:HG12	1:30:B:PHE:HA	1	1.07
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	7	1.07
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE1	7	1.07
(2,627)	1:65:B:LEU:HD21	1:85:B:LEU:H	8	1.07
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	2	1.07
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	5	1.07
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	8	1.07
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	2	1.07
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	5	1.07
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	4	1.07
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	3	1.07
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	7	1.07
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	8	1.07
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	10	1.07
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	7	1.07
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	8	1.06
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG22	3	1.06
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG21	6	1.06
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG21	7	1.06
(2,1106)	1:10:B:THR:HG22	1:71:B:ASP:HA	10	1.06
(2,959)	1:88:B:CYS:HB2	1:89:B:ILE:HG13	4	1.06
(2,959)	1:88:B:CYS:HB2	1:89:B:ILE:HG13	5	1.06
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	7	1.06
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	1	1.06
(2,564)	1:85:B:LEU:HD12	1:82:B:GLY:HA3	2	1.06
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	8	1.06
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	4	1.06
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	4	1.06
(2,169)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	10	1.06
(1,922)	1:85:B:LEU:H	1:88:B:CYS:HB3	1	1.06
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	4	1.06
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	1	1.06
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	9	1.06
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	3	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1106)	1:10:B:THR:HG21	1:71:B:ASP:HA	8	1.05
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD12	3	1.05
(2,988)	1:59:B:LYS:HB2	1:55:B:PRO:HB3	1	1.05
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	4	1.05
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB1	5	1.05
(2,643)	1:45:B:MET:HB2	1:40:B:PHE:HA	1	1.05
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	9	1.05
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	1	1.05
(2,286)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	7	1.05
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD12	4	1.05
(1,746)	1:53:B:LEU:HA	1:53:B:LEU:HD22	4	1.05
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	1	1.05
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	6	1.05
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	2	1.05
(1,485)	1:98:B:LEU:HD22	1:40:B:PHE:HB3	3	1.05
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG22	1	1.04
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD13	1	1.04
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	2	1.04
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB3	1	1.04
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	4	1.04
(2,1168)	1:54:B:ILE:HD11	1:58:B:THR:HG21	4	1.04
(2,1159)	1:45:B:MET:HG3	1:43:B:ILE:HG22	7	1.04
(2,1117)	1:-6:B:VAL:HG21	1:-4:B:ASP:H	10	1.04
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD11	1	1.04
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	2	1.04
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	8	1.04
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD21	4	1.04
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB2	9	1.04
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	10	1.04
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD22	1	1.04
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	5	1.04
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	2	1.04
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	8	1.04
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	8	1.04
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	9	1.04
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	9	1.04
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	6	1.04
(1,459)	1:85:B:LEU:HB2	1:85:B:LEU:HD23	8	1.04
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	9	1.04
(1,327)	1:81:B:TRP:HB3	1:78:B:ALA:HA	1	1.04
(1,263)	1:11:B:LYS:HB2	1:72:B:LYS:HA	9	1.04
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	5	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB2	9	1.03
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	2	1.03
(2,939)	1:34:B:PRO:HG2	1:35:B:ASP:HB2	7	1.03
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD13	6	1.03
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD11	7	1.03
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	10	1.03
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	6	1.03
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	7	1.03
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD22	9	1.03
(2,272)	1:85:B:LEU:HB3	1:19:B:THR:HA	1	1.03
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	9	1.03
(2,130)	1:40:B:PHE:HB2	1:37:B:LYS:HG3	5	1.03
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	10	1.03
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	4	1.03
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	8	1.03
(2,1494)	1:25:B:LEU:H	1:25:B:LEU:HD13	4	1.02
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	8	1.02
(2,1366)	1:11:B:LYS:H	1:13:B:ALA:HB1	3	1.02
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD13	10	1.02
(2,955)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	5	1.02
(2,937)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	7	1.02
(2,827)	1:73:B:ILE:HG22	1:74:B:ASN:HB2	5	1.02
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD12	5	1.02
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	5	1.02
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	7	1.02
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	1	1.02
(2,490)	1:81:B:TRP:HE3	1:85:B:LEU:HG	3	1.02
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	9	1.02
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD22	3	1.02
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	6	1.02
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	6	1.02
(2,140)	1:95:B:GLU:HG2	1:94:B:ALA:HB3	7	1.02
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	2	1.02
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	6	1.02
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD11	8	1.02
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	8	1.02
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD21	7	1.01
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	9	1.01
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE3	4	1.01
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	8	1.01
(2,453)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	5	1.01
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD12	10	1.01
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	4	1.01
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	3	1.01
(2,127)	1:40:B:PHE:HB3	1:31:B:ILE:HG21	9	1.01
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	5	1.01
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	5	1.01
(1,665)	1:23:B:PRO:HG2	1:55:B:PRO:HD2	7	1.01
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	4	1.0
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG23	4	1.0
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG23	10	1.0
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD11	7	1.0
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	1.0
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	2	1.0
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB2	3	1.0
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	9	1.0
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	10	1.0
(2,140)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	8	1.0
(2,140)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	10	1.0
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD11	3	1.0
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	10	1.0
(1,975)	1:62:B:GLN:H	1:63:B:ASP:HB3	5	1.0
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	8	1.0
(1,756)	1:20:B:PRO:HD3	1:21:B:LEU:HB2	1	1.0
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	8	0.99
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG21	8	0.99
(2,1168)	1:54:B:ILE:HD11	1:58:B:THR:HG21	1	0.99
(2,1117)	1:-6:B:VAL:HG12	1:-4:B:ASP:H	6	0.99
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG21	7	0.99
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	6	0.99
(2,1030)	1:44:B:LYS:HD3	1:41:B:ASP:HB2	8	0.99
(2,955)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	8	0.99
(2,651)	1:24:B:ASP:HB3	1:21:B:LEU:HD22	5	0.99
(2,628)	1:65:B:LEU:HD23	1:68:B:SER:HB2	6	0.99
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	2	0.99
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	6	0.99
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	7	0.99
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	2	0.99
(2,211)	1:38:B:LYS:HB3	1:37:B:LYS:H	7	0.99
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD11	2	0.99
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	10	0.99
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	6	0.99
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	10	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD23	2	0.99
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	9	0.99
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD23	10	0.99
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG21	6	0.98
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE2	3	0.98
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD23	4	0.98
(2,1369)	1:58:B:THR:H	1:23:B:PRO:HG2	1	0.98
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	9	0.98
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG22	9	0.98
(2,1165)	1:54:B:ILE:HD13	1:50:B:CYS:HB2	10	0.98
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG22	9	0.98
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG21	6	0.98
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	9	0.98
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	7	0.98
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD11	10	0.98
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB1	3	0.98
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB2	6	0.98
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD23	7	0.98
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	1	0.98
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	7	0.98
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	4	0.98
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	7	0.98
(2,57)	1:85:B:LEU:HB3	1:19:B:THR:HA	10	0.98
(1,569)	1:89:B:ILE:HG22	1:90:B:GLY:HA3	10	0.98
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	1	0.98
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	5	0.98
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	3	0.98
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD23	8	0.98
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	7	0.97
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	3	0.97
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	2	0.97
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	1	0.97
(2,1165)	1:54:B:ILE:HD11	1:50:B:CYS:HB2	3	0.97
(2,1165)	1:54:B:ILE:HD11	1:50:B:CYS:HB2	5	0.97
(2,1094)	1:69:B:MET:HB2	1:70:B:PRO:HA	8	0.97
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB3	2	0.97
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	1	0.97
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	8	0.97
(2,564)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	5	0.97
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	4	0.97
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	5	0.97
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	9	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	1	0.97
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	4	0.97
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD12	7	0.97
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	7	0.97
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	2	0.97
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	10	0.97
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	1	0.97
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	4	0.97
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	8	0.96
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG22	2	0.96
(2,1168)	1:54:B:ILE:HD12	1:58:B:THR:HG22	10	0.96
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG22	8	0.96
(2,1043)	1:33:B:ASP:H	1:37:B:LYS:HD3	5	0.96
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	5	0.96
(2,988)	1:60:B:LYS:HB2	1:64:B:GLU:HG2	2	0.96
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB2	10	0.96
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	1	0.96
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG21	3	0.96
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	8	0.96
(2,688)	1:38:B:LYS:HA	1:38:B:LYS:HE2	8	0.96
(2,651)	1:36:B:LEU:HD11	1:35:B:ASP:HB3	3	0.96
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	1	0.96
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	7	0.96
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	10	0.96
(2,490)	1:39:B:ARG:HG3	1:39:B:ARG:H	1	0.96
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG23	9	0.96
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	3	0.96
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	10	0.96
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	10	0.96
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	5	0.96
(2,118)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	9	0.96
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	9	0.96
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD21	3	0.96
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD2	5	0.96
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	8	0.96
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	3	0.96
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	5	0.96
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG23	9	0.95
(2,1137)	1:24:B:ASP:HA	1:25:B:LEU:HG	7	0.95
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB3	1	0.95
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD11	8	0.95
(2,872)	1:26:B:ILE:HD11	1:25:B:LEU:H	2	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD13	3	0.95
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	4	0.95
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD12	1	0.95
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	1	0.95
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	7	0.95
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	6	0.95
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	1	0.95
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	9	0.95
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB3	2	0.95
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	9	0.95
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	5	0.95
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	6	0.95
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	4	0.95
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	6	0.95
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	3	0.94
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD12	1	0.94
(2,1168)	1:54:B:ILE:HD13	1:58:B:THR:HG22	7	0.94
(2,1116)	1:19:B:THR:HG21	1:62:B:GLN:HA	8	0.94
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	8	0.94
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	9	0.94
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	5	0.94
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	9	0.94
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	10	0.94
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD13	4	0.94
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB2	4	0.94
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	5	0.94
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	5	0.94
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	8	0.94
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	7	0.94
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	8	0.94
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	6	0.93
(2,1159)	1:28:B:LYS:HB2	1:31:B:ILE:HD12	4	0.93
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB2	6	0.93
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	4	0.93
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG23	10	0.93
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	9	0.93
(2,1058)	1:92:B:ASP:HB2	1:91:B:LYS:HD3	10	0.93
(2,872)	1:26:B:ILE:HD13	1:25:B:LEU:H	6	0.93
(2,825)	1:73:B:ILE:HG22	1:18:B:MET:HG2	7	0.93
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB3	1	0.93
(2,759)	1:12:B:ASP:H	1:13:B:ALA:HB1	7	0.93
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD12	4	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	10	0.93
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	2	0.93
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	4	0.93
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB2	4	0.93
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	1	0.93
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	1	0.93
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	10	0.93
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	3	0.93
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	6	0.93
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	10	0.93
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	5	0.93
(1,667)	1:55:B:PRO:HD3	1:53:B:LEU:HA	8	0.93
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	10	0.93
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	1	0.93
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	7	0.92
(2,1165)	1:54:B:ILE:HD11	1:50:B:CYS:HB2	7	0.92
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB1	2	0.92
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG23	4	0.92
(2,1100)	1:98:B:LEU:HD13	1:39:B:ARG:H	4	0.92
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	5	0.92
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	3	0.92
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	6	0.92
(2,662)	1:77:B:THR:HG22	1:70:B:PRO:HB3	5	0.92
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	8	0.92
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	9	0.92
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	1	0.92
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	6	0.92
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	8	0.92
(2,87)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	4	0.92
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	6	0.92
(2,84)	1:12:B:ASP:HB3	1:10:B:THR:HG22	8	0.92
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	9	0.92
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB3	5	0.92
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	6	0.92
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	9	0.92
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB1	6	0.92
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	1	0.92
(2,1369)	1:58:B:THR:H	1:60:B:LYS:HD3	3	0.91
(2,1116)	1:19:B:THR:HG23	1:62:B:GLN:HA	2	0.91
(2,1103)	1:36:B:LEU:HD12	1:35:B:ASP:HB2	6	0.91
(2,774)	1:78:B:ALA:HB2	1:80:B:THR:H	8	0.91
(2,662)	1:77:B:THR:HG23	1:70:B:PRO:HB3	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,651)	1:24:B:ASP:HB3	1:21:B:LEU:HD21	1	0.91
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	6	0.91
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	7	0.91
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	8	0.91
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	10	0.91
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	4	0.91
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG23	7	0.9
(2,1494)	1:25:B:LEU:H	1:25:B:LEU:HD12	8	0.9
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	7	0.9
(2,1159)	1:28:B:LYS:HB2	1:31:B:ILE:HD12	6	0.9
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG22	9	0.9
(2,1107)	1:88:B:CYS:HA	1:89:B:ILE:HB	8	0.9
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	3	0.9
(2,1044)	1:95:B:GLU:HB2	1:96:B:LYS:HB2	10	0.9
(2,988)	1:59:B:LYS:HB2	1:55:B:PRO:HB3	3	0.9
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	3	0.9
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	10	0.9
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD23	9	0.9
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	6	0.9
(2,592)	1:44:B:LYS:HG3	1:42:B:GLU:HA	10	0.9
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	7	0.9
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	1	0.9
(2,30)	1:25:B:LEU:HB2	1:26:B:ILE:HA	8	0.9
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB2	1	0.9
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	2	0.9
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	1	0.9
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	3	0.9
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	8	0.9
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	6	0.9
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG22	2	0.89
(2,1361)	1:92:B:ASP:H	1:60:B:LYS:HE3	9	0.89
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	8	0.89
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	2	0.89
(2,1273)	1:62:B:GLN:H	1:60:B:LYS:HB2	3	0.89
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG22	8	0.89
(2,1100)	1:98:B:LEU:HD11	1:39:B:ARG:H	5	0.89
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD13	6	0.89
(2,1100)	1:99:B:ILE:H	1:98:B:LEU:HD11	9	0.89
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	9	0.89
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG23	2	0.89
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	5	0.89
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG22	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,761)	1:9:B:MET:HE3	1:9:B:MET:HA	8	0.89
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	2	0.89
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD22	8	0.89
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD22	10	0.89
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	4	0.89
(2,420)	1:81:B:TRP:HB3	1:84:B:SER:HB2	10	0.89
(2,272)	1:21:B:LEU:HB2	1:19:B:THR:HA	6	0.89
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD13	6	0.89
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	5	0.89
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD3	7	0.89
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD11	2	0.89
(2,65)	1:72:B:LYS:HE2	1:72:B:LYS:HG3	1	0.89
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	3	0.89
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	7	0.89
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	3	0.89
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	9	0.89
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	7	0.89
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	5	0.88
(2,1168)	1:54:B:ILE:HD11	1:58:B:THR:HG21	6	0.88
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	9	0.88
(2,1043)	1:33:B:ASP:H	1:37:B:LYS:HD3	4	0.88
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	8	0.88
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	6	0.88
(2,896)	1:69:B:MET:HE2	1:69:B:MET:HA	6	0.88
(2,872)	1:26:B:ILE:HD13	1:25:B:LEU:H	8	0.88
(2,827)	1:73:B:ILE:HG21	1:74:B:ASN:HB2	7	0.88
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG23	1	0.88
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	7	0.88
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	10	0.88
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG22	3	0.88
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG21	6	0.88
(2,662)	1:77:B:THR:HG22	1:70:B:PRO:HB3	9	0.88
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	6	0.88
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	2	0.88
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	5	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	4	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	7	0.88
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD12	10	0.88
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	3	0.88
(2,4)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	5	0.88
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB3	3	0.88
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	9	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	10	0.88
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	5	0.88
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	3	0.88
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	6	0.88
(1,87)	1:63:B:ASP:H	1:63:B:ASP:HB3	5	0.88
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	4	0.87
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	10	0.87
(2,1175)	1:45:B:MET:HE2	1:40:B:PHE:HD2	1	0.87
(2,1143)	1:4:B:ALA:HB2	1:5:B:ASN:HB3	4	0.87
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG23	5	0.87
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	2	0.87
(2,872)	1:26:B:ILE:HD11	1:25:B:LEU:H	5	0.87
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	9	0.87
(2,662)	1:77:B:THR:HG21	1:70:B:PRO:HB3	4	0.87
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD23	4	0.87
(2,549)	1:83:B:ARG:HG2	1:84:B:SER:HB2	5	0.87
(2,514)	1:22:B:LEU:HD22	1:82:B:GLY:HA3	4	0.87
(2,286)	1:42:B:GLU:HB2	1:39:B:ARG:HG2	5	0.87
(2,140)	1:64:B:GLU:HG3	1:60:B:LYS:HG3	1	0.87
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	2	0.87
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	9	0.87
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	8	0.87
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	1	0.87
(1,841)	1:54:B:ILE:HD12	1:23:B:PRO:HB3	10	0.87
(1,798)	1:85:B:LEU:HD21	1:64:B:GLU:H	3	0.87
(1,798)	1:85:B:LEU:HD23	1:64:B:GLU:H	9	0.87
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	4	0.87
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	3	0.87
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	6	0.87
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	1	0.87
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD11	2	0.86
(2,1165)	1:54:B:ILE:HD11	1:50:B:CYS:HB2	2	0.86
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	4	0.86
(2,1051)	1:51:B:VAL:HG22	1:48:B:GLU:HB2	8	0.86
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	6	0.86
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	8	0.86
(2,932)	1:44:B:LYS:HE2	1:44:B:LYS:HB2	9	0.86
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	5	0.86
(2,773)	1:67:B:ALA:HB3	1:68:B:SER:HA	8	0.86
(2,662)	1:77:B:THR:HG23	1:70:B:PRO:HB3	7	0.86
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	3	0.86
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB2	10	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	7	0.86
(2,525)	1:97:B:HIS:H	1:45:B:MET:HE3	5	0.86
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	8	0.86
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD12	7	0.86
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	4	0.86
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	8	0.86
(2,117)	1:50:B:CYS:HB2	1:45:B:MET:HE3	3	0.86
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	5	0.86
(2,117)	1:88:B:CYS:HB3	1:89:B:ILE:HD13	9	0.86
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	5	0.86
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	6	0.86
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	8	0.86
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	10	0.86
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	4	0.86
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD21	6	0.86
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD22	8	0.86
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	10	0.86
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	6	0.86
(1,306)	1:31:B:ILE:HG13	1:37:B:LYS:HD3	5	0.86
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	2	0.86
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	5	0.86
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	6	0.85
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	5	0.85
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	6	0.85
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB2	8	0.85
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	1	0.85
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	3	0.85
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	5	0.85
(2,932)	1:44:B:LYS:HE2	1:44:B:LYS:HB2	6	0.85
(2,905)	1:28:B:LYS:HG3	1:31:B:ILE:HD12	9	0.85
(2,827)	1:73:B:ILE:HG21	1:74:B:ASN:HB2	2	0.85
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG22	1	0.85
(2,781)	1:99:B:ILE:HG13	1:99:B:ILE:HG23	5	0.85
(2,774)	1:78:B:ALA:HB3	1:80:B:THR:H	4	0.85
(2,662)	1:77:B:THR:HG21	1:70:B:PRO:HB3	8	0.85
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	5	0.85
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	2	0.85
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	2	0.85
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	8	0.85
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	2	0.85
(2,154)	1:56:B:GLU:HG3	1:96:B:LYS:HD2	2	0.85
(2,127)	1:50:B:CYS:HB2	1:45:B:MET:HE3	3	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:93:B:PHE:HB2	1:53:B:LEU:HB2	10	0.85
(2,84)	1:12:B:ASP:HB3	1:10:B:THR:HG22	4	0.85
(2,30)	1:25:B:LEU:HB2	1:26:B:ILE:HA	4	0.85
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	4	0.85
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD22	2	0.85
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD23	10	0.85
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	2	0.85
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	7	0.85
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	1	0.85
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	7	0.85
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	7	0.85
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	2	0.84
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	7	0.84
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	7	0.84
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE1	8	0.84
(2,872)	1:26:B:ILE:HD11	1:25:B:LEU:H	7	0.84
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG21	8	0.84
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	9	0.84
(2,627)	1:65:B:LEU:HD21	1:85:B:LEU:H	5	0.84
(2,627)	1:65:B:LEU:HD23	1:85:B:LEU:H	7	0.84
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD13	3	0.84
(2,108)	1:30:B:PHE:HB2	1:36:B:LEU:HD11	10	0.84
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	1	0.84
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	7	0.84
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD12	2	0.84
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD11	3	0.84
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	10	0.84
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD1	9	0.84
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	1	0.84
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	3	0.84
(1,569)	1:89:B:ILE:HG23	1:90:B:GLY:HA3	2	0.84
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	7	0.84
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	9	0.84
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	9	0.83
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	10	0.83
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG22	3	0.83
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD11	3	0.83
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	4	0.83
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD22	5	0.83
(2,1107)	1:88:B:CYS:HA	1:89:B:ILE:HB	2	0.83
(2,1107)	1:88:B:CYS:HA	1:89:B:ILE:HB	9	0.83
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	2	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,905)	1:99:B:ILE:HD11	1:94:B:ALA:HB3	2	0.83
(2,900)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	7	0.83
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	6	0.83
(2,872)	1:29:B:GLY:H	1:26:B:ILE:HD13	1	0.83
(2,825)	1:73:B:ILE:HG23	1:9:B:MET:HE1	6	0.83
(2,715)	1:51:B:VAL:HG12	1:27:B:CYS:HB3	10	0.83
(2,662)	1:77:B:THR:HG22	1:70:B:PRO:HB3	2	0.83
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG23	3	0.83
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	4	0.83
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	3	0.83
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD22	4	0.83
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	6	0.83
(2,84)	1:71:B:ASP:HB3	1:72:B:LYS:HB3	2	0.83
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	2	0.83
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	3	0.83
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD21	5	0.83
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD23	6	0.83
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	9	0.83
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	2	0.83
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	10	0.83
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	4	0.83
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	6	0.83
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	8	0.83
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	6	0.82
(2,1304)	1:15:B:LEU:H	1:85:B:LEU:HD21	2	0.82
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	1	0.82
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	3	0.82
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	5	0.82
(2,1121)	1:60:B:LYS:HD2	1:92:B:ASP:HA	7	0.82
(2,1120)	1:99:B:ILE:HA	1:98:B:LEU:HB2	10	0.82
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	10	0.82
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE3	3	0.82
(2,825)	1:73:B:ILE:HG23	1:9:B:MET:HE1	8	0.82
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	10	0.82
(2,554)	1:73:B:ILE:HG12	1:10:B:THR:H	4	0.82
(2,322)	1:41:B:ASP:H	1:39:B:ARG:HB3	3	0.82
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	1	0.82
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	8	0.82
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	10	0.82
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	2	0.82
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	1	0.82
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB3	7	0.82
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	9	0.82
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	8	0.82
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	3	0.82
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	4	0.82
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	9	0.82
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	4	0.82
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	1	0.82
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	2	0.82
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	5	0.82
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	10	0.82
(1,87)	1:63:B:ASP:H	1:63:B:ASP:HB3	4	0.82
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	2	0.82
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	1	0.81
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	7	0.81
(2,1474)	1:63:B:ASP:H	1:59:B:LYS:HD3	9	0.81
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD23	2	0.81
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	1	0.81
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	3	0.81
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	10	0.81
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG22	10	0.81
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB1	3	0.81
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD21	5	0.81
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	7	0.81
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	1	0.81
(2,1051)	1:51:B:VAL:HG23	1:48:B:GLU:HB2	6	0.81
(2,996)	1:77:B:THR:HG23	1:70:B:PRO:HB3	7	0.81
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	10	0.81
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	5	0.81
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	9	0.81
(2,872)	1:26:B:ILE:HD13	1:25:B:LEU:H	9	0.81
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG23	3	0.81
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	8	0.81
(2,798)	1:54:B:ILE:HB	1:26:B:ILE:HG22	6	0.81
(2,761)	1:13:B:ALA:HB1	1:9:B:MET:HA	5	0.81
(2,549)	1:17:B:SER:HB2	1:9:B:MET:HE1	8	0.81
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG23	2	0.81
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	5	0.81
(2,272)	1:85:B:LEU:HB3	1:19:B:THR:HA	9	0.81
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	9	0.81
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	7	0.81
(2,29)	1:65:B:LEU:HB3	1:68:B:SER:HB2	4	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	10	0.81
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	10	0.81
(1,1266)	1:17:B:SER:H	1:15:B:LEU:HD13	5	0.81
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	10	0.81
(1,569)	1:89:B:ILE:HG21	1:90:B:GLY:HA3	9	0.81
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB3	2	0.81
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD12	2	0.81
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	8	0.81
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	10	0.81
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	1	0.81
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	5	0.81
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	9	0.81
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	10	0.81
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	8	0.8
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE1	4	0.8
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	7	0.8
(2,1120)	1:67:B:ALA:HB3	1:68:B:SER:HA	1	0.8
(2,1120)	1:99:B:ILE:HA	1:98:B:LEU:HB2	8	0.8
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG23	5	0.8
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	6	0.8
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB3	2	0.8
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD13	9	0.8
(2,985)	1:62:B:GLN:HG2	1:59:B:LYS:HD3	9	0.8
(2,975)	1:54:B:ILE:HB	1:50:B:CYS:HA	7	0.8
(2,955)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	3	0.8
(2,905)	1:99:B:ILE:HD12	1:94:B:ALA:HB3	3	0.8
(2,773)	1:67:B:ALA:HB1	1:68:B:SER:HA	10	0.8
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	2	0.8
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG22	9	0.8
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD11	9	0.8
(2,628)	1:65:B:LEU:HD21	1:68:B:SER:HB2	2	0.8
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	9	0.8
(2,585)	1:78:B:ALA:H	1:75:B:SER:HB3	8	0.8
(2,556)	1:45:B:MET:HE2	1:98:B:LEU:HA	10	0.8
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	2	0.8
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	3	0.8
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	1	0.8
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	4	0.8
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	9	0.8
(1,1295)	1:97:B:HIS:H	1:98:B:LEU:HB3	2	0.8
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	7	0.8
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD22	9	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,798)	1:85:B:LEU:HD23	1:64:B:GLU:H	7	0.8
(1,677)	1:5:B:ASN:HA	1:6:B:PRO:HD2	10	0.8
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	4	0.8
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	5	0.8
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	2	0.8
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	7	0.8
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	8	0.8
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	1	0.8
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	4	0.8
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	8	0.8
(2,1658)	1:77:B:THR:H	1:70:B:PRO:HG2	4	0.79
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD13	3	0.79
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	8	0.79
(2,1165)	1:54:B:ILE:HD12	1:50:B:CYS:HB2	1	0.79
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE2	3	0.79
(2,564)	1:85:B:LEU:HD13	1:82:B:GLY:HA3	8	0.79
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	9	0.79
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	5	0.79
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	4	0.79
(2,211)	1:67:B:ALA:H	1:69:B:MET:HG3	9	0.79
(2,178)	1:49:B:GLN:HG3	1:52:B:THR:HG23	4	0.79
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	6	0.79
(2,79)	1:35:B:ASP:H	1:35:B:ASP:HB3	5	0.79
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	4	0.79
(1,841)	1:54:B:ILE:HD11	1:23:B:PRO:HB3	6	0.79
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	7	0.79
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB3	3	0.79
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	1	0.79
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	7	0.79
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	2	0.79
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	5	0.79
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	6	0.79
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG22	4	0.78
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD12	6	0.78
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	9	0.78
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	2	0.78
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	8	0.78
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	7	0.78
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD12	3	0.78
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	1	0.78
(2,955)	1:8:B:GLU:HB3	1:7:B:ASN:HB3	4	0.78
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	2	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,921)	1:84:B:SER:HB2	1:81:B:TRP:HZ3	6	0.78
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	9	0.78
(2,761)	1:13:B:ALA:HB2	1:9:B:MET:HA	6	0.78
(2,761)	1:13:B:ALA:HB2	1:9:B:MET:HA	9	0.78
(2,662)	1:77:B:THR:HG22	1:70:B:PRO:HB3	10	0.78
(2,322)	1:41:B:ASP:H	1:39:B:ARG:HB3	7	0.78
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	7	0.78
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	1	0.78
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	9	0.78
(2,84)	1:12:B:ASP:HB3	1:10:B:THR:HG21	5	0.78
(2,4)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	7	0.78
(1,1013)	1:50:B:CYS:H	1:53:B:LEU:HD23	7	0.78
(1,941)	1:87:B:GLU:H	1:88:B:CYS:HB3	1	0.78
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	6	0.78
(1,798)	1:85:B:LEU:HD23	1:64:B:GLU:H	4	0.78
(1,798)	1:85:B:LEU:HD22	1:64:B:GLU:H	5	0.78
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	7	0.78
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	3	0.78
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	6	0.78
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	4	0.78
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	5	0.78
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	6	0.78
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	7	0.77
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG23	1	0.77
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG23	2	0.77
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG21	9	0.77
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB1	9	0.77
(2,1120)	1:67:B:ALA:HB3	1:68:B:SER:HA	3	0.77
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	3	0.77
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	7	0.77
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	7	0.77
(2,1030)	1:54:B:ILE:HG12	1:27:B:CYS:HB3	3	0.77
(2,984)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	10	0.77
(2,943)	1:35:B:ASP:HB3	1:38:B:LYS:HG2	9	0.77
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	1	0.77
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD2	8	0.77
(2,822)	1:73:B:ILE:HG21	1:11:B:LYS:HA	4	0.77
(2,774)	1:78:B:ALA:HB2	1:80:B:THR:H	1	0.77
(2,774)	1:78:B:ALA:HB3	1:80:B:THR:H	9	0.77
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG23	1	0.77
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG23	5	0.77
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	7	0.77
(2,549)	1:17:B:SER:HB2	1:9:B:MET:HE1	2	0.77
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	8	0.77
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	4	0.77
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	10	0.77
(2,236)	1:9:B:MET:HG2	1:72:B:LYS:HB3	10	0.77
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	7	0.77
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	8	0.77
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	5	0.77
(2,200)	1:69:B:MET:HB2	1:11:B:LYS:HA	2	0.77
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD2	3	0.77
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	3	0.77
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	4	0.77
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	8	0.77
(1,754)	1:37:B:LYS:H	1:33:B:ASP:HB2	6	0.77
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	8	0.77
(1,321)	1:81:B:TRP:HB2	1:81:B:TRP:HE3	2	0.77
(1,214)	1:34:B:PRO:HB3	1:34:B:PRO:HD2	10	0.77
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	8	0.77
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	9	0.77
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	6	0.76
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	3	0.76
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD13	9	0.76
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD23	9	0.76
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD21	10	0.76
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD13	7	0.76
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG22	8	0.76
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	6	0.76
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG22	7	0.76
(2,1114)	1:49:B:GLN:H	1:46:B:THR:HG22	3	0.76
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB1	5	0.76
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	6	0.76
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	1	0.76
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	9	0.76
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	10	0.76
(2,773)	1:67:B:ALA:HB3	1:68:B:SER:HA	1	0.76
(2,761)	1:9:B:MET:HE3	1:9:B:MET:HA	10	0.76
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD13	2	0.76
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD23	4	0.76
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	8	0.76
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	4	0.76
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD13	7	0.76
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	2	0.76
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE2	3	0.76
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	6	0.76
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	3	0.76
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	3	0.76
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	6	0.76
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD11	1	0.76
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD13	2	0.76
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	2	0.76
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	1	0.76
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	2	0.76
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	9	0.76
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	8	0.76
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	3	0.76
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	1	0.75
(2,1556)	1:96:B:LYS:H	1:99:B:ILE:HG23	8	0.75
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD13	4	0.75
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD21	3	0.75
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD22	8	0.75
(2,1273)	1:62:B:GLN:H	1:59:B:LYS:HB3	5	0.75
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD21	4	0.75
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	5	0.75
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	2	0.75
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD22	9	0.75
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	4	0.75
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	10	0.75
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	4	0.75
(2,975)	1:54:B:ILE:HB	1:50:B:CYS:HA	2	0.75
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD21	2	0.75
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	1	0.75
(2,774)	1:78:B:ALA:HB1	1:80:B:THR:H	7	0.75
(2,774)	1:78:B:ALA:HB1	1:80:B:THR:H	10	0.75
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	10	0.75
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD12	10	0.75
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG23	10	0.75
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD12	2	0.75
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	1	0.75
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	10	0.75
(2,341)	1:38:B:LYS:HD2	1:38:B:LYS:HA	3	0.75
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD12	10	0.75
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	9	0.75
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	5	0.75
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD11	5	0.75
(1,455)	1:85:B:LEU:HD21	1:85:B:LEU:H	6	0.75
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	8	0.75
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	2	0.74
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	5	0.74
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	10	0.74
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	9	0.74
(2,1120)	1:67:B:ALA:HB3	1:68:B:SER:HA	9	0.74
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE2	3	0.74
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	5	0.74
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	2	0.74
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	9	0.74
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	2	0.74
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	1	0.74
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG21	4	0.74
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	6	0.74
(2,825)	1:73:B:ILE:HG22	1:9:B:MET:HE3	5	0.74
(2,802)	1:26:B:ILE:HG22	1:86:B:GLY:HA2	3	0.74
(2,776)	1:31:B:ILE:HG22	1:40:B:PHE:HE1	1	0.74
(2,664)	1:57:B:SER:H	1:58:B:THR:HG21	5	0.74
(2,662)	1:77:B:THR:HG21	1:70:B:PRO:HB3	3	0.74
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD21	5	0.74
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	8	0.74
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	9	0.74
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	4	0.74
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	2	0.74
(2,282)	1:18:B:MET:HG2	1:21:B:LEU:HD11	3	0.74
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	6	0.74
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	9	0.74
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	10	0.74
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD13	2	0.74
(2,104)	1:30:B:PHE:HB3	1:30:B:PHE:HE1	3	0.74
(1,1336)	1:90:B:GLY:H	1:91:B:LYS:HG3	5	0.74
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	6	0.74
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	6	0.74
(1,812)	1:80:B:THR:HG22	1:81:B:TRP:HZ2	1	0.74
(1,628)	1:98:B:LEU:HB3	1:94:B:ALA:HA	4	0.74
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	1	0.74
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	2	0.74
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	3	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	4	0.74
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	9	0.74
(1,11)	1:53:B:LEU:HB3	1:53:B:LEU:HD12	4	0.74
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	4	0.73
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	9	0.73
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD13	10	0.73
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD11	2	0.73
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	5	0.73
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	5	0.73
(2,1159)	1:45:B:MET:HG3	1:43:B:ILE:HG21	9	0.73
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	6	0.73
(2,1117)	1:-6:B:VAL:HG21	1:-4:B:ASP:H	7	0.73
(2,1103)	1:36:B:LEU:HD12	1:35:B:ASP:HB2	4	0.73
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	7	0.73
(2,1091)	1:14:B:TRP:HA	1:13:B:ALA:HB2	9	0.73
(2,1051)	1:51:B:VAL:HG21	1:48:B:GLU:HB2	2	0.73
(2,1023)	1:89:B:ILE:HG13	1:61:B:CYS:HA	7	0.73
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	1	0.73
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	2	0.73
(2,827)	1:73:B:ILE:HG23	1:74:B:ASN:HB2	6	0.73
(2,801)	1:89:B:ILE:HD13	1:86:B:GLY:HA3	5	0.73
(2,774)	1:78:B:ALA:HB2	1:80:B:THR:H	3	0.73
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	7	0.73
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG21	3	0.73
(2,662)	1:77:B:THR:HG23	1:70:B:PRO:HB3	6	0.73
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	6	0.73
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	2	0.73
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD12	3	0.73
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD12	5	0.73
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	1	0.73
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	4	0.73
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	5	0.73
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	6	0.73
(2,228)	1:38:B:LYS:H	1:37:B:LYS:HB2	10	0.73
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	7	0.73
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HB	5	0.73
(1,1296)	1:97:B:HIS:H	1:94:B:ALA:HB1	4	0.73
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD13	4	0.73
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	7	0.73
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	9	0.73
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD2	3	0.73
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:30:B:PHE:HB3	1:31:B:ILE:HG12	1	0.73
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	2	0.73
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	5	0.73
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	7	0.73
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	8	0.73
(1,36)	1:85:B:LEU:H	1:85:B:LEU:HB3	10	0.73
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD13	2	0.72
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	7	0.72
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	9	0.72
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	3	0.72
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD12	1	0.72
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD12	8	0.72
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	7	0.72
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG21	2	0.72
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	4	0.72
(2,1051)	1:51:B:VAL:HG23	1:48:B:GLU:HB2	10	0.72
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	7	0.72
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	10	0.72
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	1	0.72
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG23	6	0.72
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG23	7	0.72
(2,778)	1:31:B:ILE:HG23	1:32:B:GLN:HG3	1	0.72
(2,776)	1:31:B:ILE:HG22	1:40:B:PHE:HE1	10	0.72
(2,773)	1:67:B:ALA:HB3	1:68:B:SER:HA	3	0.72
(2,664)	1:57:B:SER:H	1:58:B:THR:HG21	4	0.72
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG21	8	0.72
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	9	0.72
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD11	3	0.72
(2,652)	1:36:B:LEU:H	1:36:B:LEU:HD13	8	0.72
(2,592)	1:72:B:LYS:HG2	1:71:B:ASP:HA	5	0.72
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	6	0.72
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	8	0.72
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	10	0.72
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE3	4	0.72
(2,467)	1:39:B:ARG:HG2	1:98:B:LEU:HB2	9	0.72
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	4	0.72
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	1	0.72
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	9	0.72
(2,140)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	5	0.72
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	1	0.72
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD13	3	0.72
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	9	0.72
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	10	0.72
(1,485)	1:98:B:LEU:HD22	1:40:B:PHE:HB3	1	0.72
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	6	0.72
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	6	0.71
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	10	0.71
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	2	0.71
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG22	1	0.71
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD21	5	0.71
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD21	8	0.71
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	1	0.71
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	3	0.71
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	10	0.71
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE3	10	0.71
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	3	0.71
(2,1020)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	3	0.71
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	2	0.71
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	3	0.71
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	2	0.71
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	4	0.71
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	9	0.71
(2,822)	1:73:B:ILE:HG22	1:11:B:LYS:HA	7	0.71
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	2	0.71
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	10	0.71
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD13	4	0.71
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	2	0.71
(2,322)	1:41:B:ASP:H	1:39:B:ARG:HB3	10	0.71
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE1	8	0.71
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	10	0.71
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	4	0.71
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	4	0.71
(2,128)	1:40:B:PHE:HB2	1:36:B:LEU:HA	1	0.71
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	2	0.71
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	6	0.71
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	10	0.71
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG11	7	0.71
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	5	0.71
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	5	0.71
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	2	0.71
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD13	1	0.71
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	10	0.71
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:61:B:CYS:HB3	1:88:B:CYS:HB3	1	0.71
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	9	0.71
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	10	0.71
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	1	0.7
(2,1506)	1:16:B:ASN:H	1:15:B:LEU:HD22	7	0.7
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	5	0.7
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	6	0.7
(2,1045)	1:23:B:PRO:HG2	1:54:B:ILE:HG22	7	0.7
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	3	0.7
(2,1009)	1:66:B:TYR:HA	1:11:B:LYS:HB3	3	0.7
(2,975)	1:54:B:ILE:HB	1:50:B:CYS:HA	6	0.7
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	8	0.7
(2,802)	1:26:B:ILE:HG21	1:86:B:GLY:HA2	2	0.7
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	2	0.7
(2,773)	1:67:B:ALA:HB3	1:68:B:SER:HA	9	0.7
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	2	0.7
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG22	5	0.7
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	5	0.7
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	5	0.7
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	5	0.7
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD22	9	0.7
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE1	2	0.7
(2,200)	1:69:B:MET:HB2	1:11:B:LYS:HA	1	0.7
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	9	0.7
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	7	0.7
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	7	0.7
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	10	0.7
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG21	10	0.7
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	2	0.7
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	2	0.7
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG21	3	0.7
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	10	0.7
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	6	0.7
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD2	9	0.7
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	6	0.7
(1,116)	1:88:B:CYS:H	1:88:B:CYS:HB3	1	0.7
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	2	0.69
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD13	9	0.69
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	3	0.69
(2,1329)	1:94:B:ALA:H	1:97:B:HIS:HB2	3	0.69
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD21	10	0.69
(2,1216)	1:13:B:ALA:H	1:17:B:SER:HB2	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG22	7	0.69
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB1	10	0.69
(2,1051)	1:51:B:VAL:HG22	1:48:B:GLU:HB2	1	0.69
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	6	0.69
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	8	0.69
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	8	0.69
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	3	0.69
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE2	3	0.69
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD22	3	0.69
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE2	6	0.69
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	2	0.69
(2,822)	1:73:B:ILE:HG22	1:11:B:LYS:HA	2	0.69
(2,822)	1:73:B:ILE:HG23	1:11:B:LYS:HA	3	0.69
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG21	7	0.69
(2,761)	1:9:B:MET:HE1	1:9:B:MET:HA	3	0.69
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG22	2	0.69
(2,638)	1:43:B:ILE:HG12	1:98:B:LEU:HD21	9	0.69
(2,549)	1:83:B:ARG:HG2	1:84:B:SER:HB2	6	0.69
(2,528)	1:22:B:LEU:HD23	1:86:B:GLY:HA3	5	0.69
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG21	1	0.69
(2,486)	1:57:B:SER:HB2	1:54:B:ILE:HG23	8	0.69
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD11	5	0.69
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD13	10	0.69
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	9	0.69
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	10	0.69
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	2	0.69
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	5	0.69
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	4	0.69
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	10	0.69
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD21	4	0.69
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	1	0.69
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	6	0.69
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	7	0.69
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	3	0.69
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	6	0.69
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	7	0.69
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD12	5	0.68
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD11	6	0.68
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	8	0.68
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	3	0.68
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	7	0.68
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	3	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HZ3	9	0.68
(2,1139)	1:92:B:ASP:H	1:89:B:ILE:HG21	6	0.68
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	5	0.68
(2,1113)	1:49:B:GLN:H	1:46:B:THR:HG22	3	0.68
(2,1096)	1:39:B:ARG:HD2	1:98:B:LEU:HD12	10	0.68
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	2	0.68
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG22	5	0.68
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	4	0.68
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	10	0.68
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	4	0.68
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG23	6	0.68
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	9	0.68
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	6	0.68
(2,545)	1:17:B:SER:HB3	1:14:B:TRP:HD1	4	0.68
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	9	0.68
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	1	0.68
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	7	0.68
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	3	0.68
(2,434)	1:51:B:VAL:HA	1:54:B:ILE:HA	5	0.68
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	9	0.68
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	3	0.68
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	3	0.68
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG23	9	0.68
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	6	0.68
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	2	0.68
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	8	0.68
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG21	7	0.68
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD1	2	0.68
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB2	1	0.68
(1,253)	1:23:B:PRO:HB3	1:55:B:PRO:HD2	7	0.68
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	9	0.68
(1,28)	1:26:B:ILE:H	1:25:B:LEU:HB2	8	0.68
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD13	8	0.67
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD23	6	0.67
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	2	0.67
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	8	0.67
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	9	0.67
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	4	0.67
(2,1143)	1:4:B:ALA:HB1	1:5:B:ASN:HB3	10	0.67
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	7	0.67
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG21	4	0.67
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	8	0.67
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	10	0.67
(2,1045)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	10	0.67
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	4	0.67
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	8	0.67
(2,928)	1:65:B:LEU:HB3	1:85:B:LEU:HD12	7	0.67
(2,915)	1:26:B:ILE:HG21	1:27:B:CYS:HB2	5	0.67
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG21	2	0.67
(2,801)	1:89:B:ILE:HD13	1:86:B:GLY:HA3	4	0.67
(2,801)	1:89:B:ILE:HD12	1:86:B:GLY:HA3	8	0.67
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE1	5	0.67
(2,774)	1:78:B:ALA:HB3	1:80:B:THR:H	6	0.67
(2,715)	1:51:B:VAL:HG12	1:27:B:CYS:HB3	6	0.67
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	8	0.67
(2,688)	1:38:B:LYS:HA	1:38:B:LYS:HE3	3	0.67
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	1	0.67
(2,514)	1:22:B:LEU:HD23	1:82:B:GLY:HA3	3	0.67
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	4	0.67
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	4	0.67
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD13	8	0.67
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	1	0.67
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	4	0.67
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	5	0.67
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	4	0.67
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD11	6	0.67
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	7	0.67
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD11	4	0.67
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	10	0.67
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	8	0.67
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	9	0.67
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	1	0.67
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG22	8	0.67
(1,841)	1:54:B:ILE:HD11	1:23:B:PRO:HB3	1	0.67
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	3	0.67
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	6	0.67
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	10	0.67
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	4	0.66
(2,1359)	1:58:B:THR:H	1:59:B:LYS:HG3	4	0.66
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD23	1	0.66
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	6	0.66
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	1	0.66
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	6	0.66
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	8	0.66
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	1	0.66
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	7	0.66
(2,972)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	2	0.66
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	6	0.66
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD21	1	0.66
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD13	1	0.66
(2,849)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	5	0.66
(2,778)	1:31:B:ILE:HG22	1:32:B:GLN:HG3	7	0.66
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG22	10	0.66
(2,651)	1:33:B:ASP:HB3	1:36:B:LEU:HD12	7	0.66
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	5	0.66
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	9	0.66
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.66
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	1	0.66
(2,221)	1:69:B:MET:HB2	1:67:B:ALA:HA	6	0.66
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD21	8	0.66
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HB	4	0.66
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	1	0.66
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	8	0.66
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	8	0.66
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	6	0.66
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	2	0.66
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD11	1	0.65
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG22	9	0.65
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	5	0.65
(2,1506)	1:16:B:ASN:H	1:15:B:LEU:HD21	8	0.65
(2,1506)	1:16:B:ASN:H	1:15:B:LEU:HD22	9	0.65
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	1	0.65
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	4	0.65
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	5	0.65
(2,1502)	1:38:B:LYS:H	1:37:B:LYS:HB2	6	0.65
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	5	0.65
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	7	0.65
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	4	0.65
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD11	6	0.65
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD12	10	0.65
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	5	0.65
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	4	0.65
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD12	3	0.65
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1116)	1:19:B:THR:HG22	1:62:B:GLN:HA	9	0.65
(2,1116)	1:19:B:THR:HG23	1:62:B:GLN:HA	10	0.65
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	2	0.65
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	5	0.65
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	7	0.65
(2,1043)	1:48:B:GLU:HB3	1:52:B:THR:H	1	0.65
(2,1020)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	6	0.65
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	1	0.65
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	9	0.65
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	4	0.65
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	8	0.65
(2,961)	1:50:B:CYS:HB3	1:54:B:ILE:HG12	5	0.65
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	8	0.65
(2,929)	1:61:B:CYS:HB2	1:57:B:SER:HB3	6	0.65
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	4	0.65
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE2	5	0.65
(2,884)	1:90:B:GLY:HA3	1:94:B:ALA:HB2	5	0.65
(2,857)	1:23:B:PRO:HD2	1:54:B:ILE:HG22	9	0.65
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG21	4	0.65
(2,608)	1:85:B:LEU:HD22	1:62:B:GLN:HB2	6	0.65
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD23	7	0.65
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	3	0.65
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	7	0.65
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	8	0.65
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	2	0.65
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	6	0.65
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	8	0.65
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	1	0.65
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD3	5	0.65
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	5	0.65
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	3	0.65
(2,169)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	9	0.65
(2,38)	1:60:B:LYS:HE2	1:60:B:LYS:HB2	9	0.65
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	10	0.65
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG21	1	0.65
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	7	0.65
(1,197)	1:61:B:CYS:H	1:60:B:LYS:HB2	9	0.65
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	7	0.65
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	8	0.65
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	2	0.65
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	4	0.65
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	2	0.65
(1,28)	1:26:B:ILE:H	1:25:B:LEU:HB2	4	0.65
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD13	5	0.64
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD12	10	0.64
(2,1502)	1:38:B:LYS:H	1:38:B:LYS:HD2	8	0.64
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG21	6	0.64
(2,1474)	1:63:B:ASP:H	1:59:B:LYS:HD3	5	0.64
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD13	9	0.64
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD22	1	0.64
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	2	0.64
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG23	6	0.64
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	9	0.64
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	8	0.64
(2,1084)	1:53:B:LEU:HD13	1:96:B:LYS:HD3	2	0.64
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	8	0.64
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	3	0.64
(2,1043)	1:49:B:GLN:HB3	1:52:B:THR:H	2	0.64
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	5	0.64
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	5	0.64
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG23	3	0.64
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG23	6	0.64
(2,774)	1:78:B:ALA:HB2	1:80:B:THR:H	2	0.64
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	5	0.64
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	8	0.64
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG21	4	0.64
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	7	0.64
(2,606)	1:86:B:GLY:H	1:85:B:LEU:HD22	5	0.64
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE2	10	0.64
(2,560)	1:72:B:LYS:H	1:73:B:ILE:HG12	3	0.64
(2,556)	1:45:B:MET:HE2	1:45:B:MET:HA	5	0.64
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	3	0.64
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	3	0.64
(2,412)	1:26:B:ILE:HG13	1:86:B:GLY:HA2	3	0.64
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	8	0.64
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	1	0.64
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	4	0.64
(2,29)	1:25:B:LEU:HB2	1:22:B:LEU:HA	8	0.64
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	7	0.64
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	1	0.64
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	8	0.64
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	2	0.64
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	1	0.64
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	4	0.64
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	8	0.64
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD13	7	0.63
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	3	0.63
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	1	0.63
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG22	4	0.63
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	8	0.63
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	5	0.63
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD12	7	0.63
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	3	0.63
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	9	0.63
(2,1304)	1:15:B:LEU:H	1:85:B:LEU:HD21	1	0.63
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD11	9	0.63
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	6	0.63
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB3	1	0.63
(2,1142)	1:9:B:MET:HG3	1:78:B:ALA:HB1	6	0.63
(2,1120)	1:67:B:ALA:HB2	1:68:B:SER:HA	4	0.63
(2,1116)	1:19:B:THR:HG21	1:62:B:GLN:HA	7	0.63
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	1	0.63
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	6	0.63
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	6	0.63
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	1	0.63
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD12	7	0.63
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE1	1	0.63
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE1	2	0.63
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	4	0.63
(2,810)	1:89:B:ILE:H	1:89:B:ILE:HD12	10	0.63
(2,664)	1:57:B:SER:H	1:58:B:THR:HG21	1	0.63
(2,651)	1:33:B:ASP:HB3	1:36:B:LEU:HD11	6	0.63
(2,607)	1:65:B:LEU:H	1:85:B:LEU:HD21	3	0.63
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	4	0.63
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	8	0.63
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	8	0.63
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	5	0.63
(2,200)	1:69:B:MET:HB2	1:11:B:LYS:HA	10	0.63
(2,154)	1:56:B:GLU:HG3	1:53:B:LEU:HB3	3	0.63
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	8	0.63
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	8	0.63
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	3	0.63
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	4	0.63
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	10	0.63
(1,841)	1:54:B:ILE:HD13	1:23:B:PRO:HB3	7	0.63
(1,690)	1:26:B:ILE:HD11	1:30:B:PHE:HE2	3	0.63
(1,574)	1:78:B:ALA:HB2	1:77:B:THR:H	3	0.63
(1,485)	1:98:B:LEU:HD23	1:40:B:PHE:HB3	8	0.63
(1,439)	1:64:B:GLU:HB3	1:65:B:LEU:HD13	3	0.63
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	2	0.63
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	5	0.63
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	5	0.63
(1,111)	1:51:B:VAL:H	1:50:B:CYS:HB2	3	0.63
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG11	1	0.63
(1,15)	1:33:B:ASP:HB2	1:36:B:LEU:HB2	6	0.63
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	9	0.62
(2,1506)	1:95:B:GLU:H	1:98:B:LEU:HD11	4	0.62
(2,1478)	1:27:B:CYS:H	1:54:B:ILE:HG22	9	0.62
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	6	0.62
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD13	3	0.62
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD23	3	0.62
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	10	0.62
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	9	0.62
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB2	10	0.62
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD13	1	0.62
(2,1051)	1:51:B:VAL:HG23	1:48:B:GLU:HB2	4	0.62
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	5	0.62
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	3	0.62
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	7	0.62
(2,915)	1:26:B:ILE:HG23	1:27:B:CYS:HB2	3	0.62
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD11	5	0.62
(2,890)	1:11:B:LYS:H	1:69:B:MET:HE2	3	0.62
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE3	8	0.62
(2,778)	1:31:B:ILE:HG22	1:32:B:GLN:HG3	6	0.62
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	3	0.62
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG23	7	0.62
(2,606)	1:85:B:LEU:HD21	1:66:B:TYR:H	8	0.62
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	5	0.62
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	3	0.62
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	10	0.62
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD23	7	0.62
(2,151)	1:76:B:GLU:HG2	1:80:B:THR:HG21	5	0.62
(2,140)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	2	0.62
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HB	8	0.62
(2,16)	1:92:B:ASP:HB2	1:60:B:LYS:HD2	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	10	0.62
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	3	0.62
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	5	0.62
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD23	4	0.62
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE1	7	0.62
(1,574)	1:78:B:ALA:HB2	1:77:B:THR:H	1	0.62
(1,574)	1:78:B:ALA:HB2	1:77:B:THR:H	2	0.62
(1,574)	1:78:B:ALA:HB1	1:77:B:THR:H	5	0.62
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	2	0.62
(1,111)	1:51:B:VAL:H	1:50:B:CYS:HB2	5	0.62
(2,1613)	1:31:B:ILE:H	1:31:B:ILE:HD13	3	0.61
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG23	5	0.61
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	2	0.61
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	3	0.61
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	10	0.61
(2,1304)	1:15:B:LEU:H	1:69:B:MET:HG2	9	0.61
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD21	3	0.61
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	10	0.61
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	7	0.61
(2,1084)	1:53:B:LEU:HD11	1:96:B:LYS:HD3	5	0.61
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	6	0.61
(2,1023)	1:89:B:ILE:HG13	1:88:B:CYS:HA	1	0.61
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	6	0.61
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	10	0.61
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	8	0.61
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	10	0.61
(2,985)	1:62:B:GLN:HG3	1:59:B:LYS:HD3	5	0.61
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	4	0.61
(2,943)	1:35:B:ASP:HB3	1:38:B:LYS:HG2	6	0.61
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	10	0.61
(2,894)	1:14:B:TRP:HB3	1:69:B:MET:HE1	2	0.61
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG21	5	0.61
(2,801)	1:89:B:ILE:HD12	1:86:B:GLY:HA3	1	0.61
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	7	0.61
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE2	4	0.61
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	2	0.61
(2,495)	1:81:B:TRP:HE3	1:85:B:LEU:HG	3	0.61
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	9	0.61
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	5	0.61
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	2	0.61
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	7	0.61
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD11	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	5	0.61
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD21	1	0.61
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD21	3	0.61
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG2	1	0.61
(2,58)	1:85:B:LEU:HB3	1:88:B:CYS:H	5	0.61
(1,1109)	1:41:B:ASP:H	1:43:B:ILE:HD12	9	0.61
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	5	0.61
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	1	0.61
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	10	0.61
(1,574)	1:78:B:ALA:HB3	1:77:B:THR:H	9	0.61
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	7	0.61
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	3	0.61
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	3	0.61
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	2	0.61
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	4	0.6
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	5	0.6
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD11	7	0.6
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	1	0.6
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	10	0.6
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	8	0.6
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD22	8	0.6
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	7	0.6
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	8	0.6
(2,1313)	1:66:B:TYR:H	1:66:B:TYR:HD2	5	0.6
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB3	3	0.6
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	2	0.6
(2,1121)	1:92:B:ASP:HA	1:94:B:ALA:HB2	4	0.6
(2,1078)	1:65:B:LEU:HD12	1:88:B:CYS:H	9	0.6
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	3	0.6
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	1	0.6
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	10	0.6
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	7	0.6
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD12	6	0.6
(2,905)	1:99:B:ILE:HD13	1:94:B:ALA:HB1	4	0.6
(2,896)	1:73:B:ILE:HD12	1:69:B:MET:HA	8	0.6
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD12	8	0.6
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE1	5	0.6
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	2	0.6
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG23	7	0.6
(2,801)	1:89:B:ILE:HD12	1:86:B:GLY:HA3	10	0.6
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG22	9	0.6
(2,778)	1:99:B:ILE:HG23	1:95:B:GLU:HG2	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,762)	1:13:B:ALA:HB1	1:14:B:TRP:HB2	7	0.6
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	6	0.6
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	7	0.6
(2,468)	1:39:B:ARG:HG2	1:39:B:ARG:HA	4	0.6
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD11	9	0.6
(2,391)	1:48:B:GLU:HB3	1:47:B:TYR:HD2	9	0.6
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	4	0.6
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	6	0.6
(2,341)	1:38:B:LYS:HD3	1:38:B:LYS:HA	2	0.6
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	8	0.6
(2,155)	1:95:B:GLU:HG3	1:99:B:ILE:HG12	8	0.6
(1,841)	1:54:B:ILE:HD13	1:23:B:PRO:HB3	5	0.6
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	8	0.6
(1,812)	1:80:B:THR:HG21	1:81:B:TRP:HZ2	7	0.6
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	9	0.6
(1,574)	1:78:B:ALA:HB3	1:77:B:THR:H	4	0.6
(1,574)	1:78:B:ALA:HB1	1:77:B:THR:H	10	0.6
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	3	0.6
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	10	0.6
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	3	0.6
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG13	10	0.6
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	1	0.59
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	4	0.59
(2,1361)	1:92:B:ASP:H	1:91:B:LYS:HE3	8	0.59
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	3	0.59
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG22	4	0.59
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	10	0.59
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	3	0.59
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HZ3	1	0.59
(2,1144)	1:17:B:SER:HB2	1:13:B:ALA:HB1	6	0.59
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB2	10	0.59
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB1	8	0.59
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	6	0.59
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG22	7	0.59
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	1	0.59
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	4	0.59
(2,985)	1:62:B:GLN:HG2	1:59:B:LYS:HD3	4	0.59
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	10	0.59
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	10	0.59
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE3	6	0.59
(2,822)	1:73:B:ILE:HG23	1:11:B:LYS:HA	5	0.59
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG21	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:45:B:MET:HE3	1:98:B:LEU:HA	6	0.59
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	1	0.59
(2,545)	1:17:B:SER:HB3	1:14:B:TRP:HD1	6	0.59
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	1	0.59
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD2	2	0.59
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	3	0.59
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	6	0.59
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	9	0.59
(2,371)	1:44:B:LYS:HD3	1:44:B:LYS:HB3	10	0.59
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	3	0.59
(2,341)	1:38:B:LYS:HD2	1:38:B:LYS:HA	7	0.59
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	6	0.59
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	1	0.59
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD12	9	0.59
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	2	0.59
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	8	0.59
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	7	0.59
(1,574)	1:78:B:ALA:HB3	1:77:B:THR:H	6	0.59
(1,574)	1:78:B:ALA:HB1	1:77:B:THR:H	7	0.59
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	4	0.59
(1,58)	1:36:B:LEU:HB2	1:30:B:PHE:HB2	3	0.59
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	8	0.59
(2,1476)	1:65:B:LEU:H	1:85:B:LEU:HD21	6	0.58
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD11	2	0.58
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD13	5	0.58
(2,1456)	1:93:B:PHE:H	1:96:B:LYS:HB2	7	0.58
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	1	0.58
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	6	0.58
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD23	1	0.58
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG23	2	0.58
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG22	6	0.58
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	7	0.58
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	3	0.58
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD21	6	0.58
(2,1211)	1:33:B:ASP:H	1:31:B:ILE:HG23	10	0.58
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	6	0.58
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB3	8	0.58
(2,1159)	1:45:B:MET:HG3	1:43:B:ILE:HG21	10	0.58
(2,1157)	1:73:B:ILE:HG21	1:14:B:TRP:HZ3	8	0.58
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE1	10	0.58
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB1	4	0.58
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	1	0.58
(2,1045)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	2	0.58
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD22	5	0.58
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	2	0.58
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	3	0.58
(2,882)	1:93:B:PHE:HB3	1:90:B:GLY:HA3	7	0.58
(2,810)	1:89:B:ILE:H	1:89:B:ILE:HD11	6	0.58
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	6	0.58
(2,774)	1:78:B:ALA:HB1	1:80:B:THR:H	5	0.58
(2,773)	1:67:B:ALA:HB2	1:68:B:SER:HA	4	0.58
(2,712)	1:51:B:VAL:HG13	1:47:B:TYR:HE1	7	0.58
(2,664)	1:57:B:SER:H	1:58:B:THR:HG22	8	0.58
(2,664)	1:57:B:SER:H	1:58:B:THR:HG23	9	0.58
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	1	0.58
(2,630)	1:15:B:LEU:HD11	1:15:B:LEU:HA	2	0.58
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE3	7	0.58
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	2	0.58
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	6	0.58
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	7	0.58
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	4	0.58
(2,430)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	10	0.58
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	2	0.58
(2,200)	1:69:B:MET:HB2	1:67:B:ALA:HA	6	0.58
(2,178)	1:49:B:GLN:HG3	1:52:B:THR:HG22	9	0.58
(2,104)	1:30:B:PHE:HB3	1:30:B:PHE:HE1	5	0.58
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	1	0.58
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	5	0.58
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	6	0.58
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	7	0.58
(1,574)	1:78:B:ALA:HB2	1:77:B:THR:H	8	0.58
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	10	0.58
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	10	0.58
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	10	0.58
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	4	0.58
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	8	0.57
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG23	1	0.57
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	2	0.57
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	6	0.57
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	6	0.57
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD13	10	0.57
(2,1422)	1:41:B:ASP:H	1:44:B:LYS:HG3	10	0.57
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1276)	1:62:B:GLN:H	1:15:B:LEU:HD23	2	0.57
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB1	10	0.57
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB2	8	0.57
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	1	0.57
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	4	0.57
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE2	4	0.57
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	4	0.57
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	3	0.57
(2,1055)	1:32:B:GLN:H	1:31:B:ILE:HG12	9	0.57
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	10	0.57
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	6	0.57
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	10	0.57
(2,943)	1:35:B:ASP:HB3	1:38:B:LYS:HG2	10	0.57
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD23	8	0.57
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD22	10	0.57
(2,896)	1:73:B:ILE:HD11	1:69:B:MET:HA	5	0.57
(2,888)	1:73:B:ILE:H	1:73:B:ILE:HD11	2	0.57
(2,888)	1:73:B:ILE:H	1:73:B:ILE:HD12	7	0.57
(2,874)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	10	0.57
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG23	1	0.57
(2,825)	1:73:B:ILE:HG21	1:9:B:MET:HE3	9	0.57
(2,810)	1:58:B:THR:H	1:89:B:ILE:HD11	1	0.57
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG21	2	0.57
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG22	3	0.57
(2,772)	1:13:B:ALA:HB3	1:16:B:ASN:HB3	3	0.57
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD13	1	0.57
(2,630)	1:15:B:LEU:HD12	1:15:B:LEU:HA	5	0.57
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	10	0.57
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	1	0.57
(2,583)	1:21:B:LEU:HD11	1:17:B:SER:HB3	6	0.57
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	7	0.57
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE2	9	0.57
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD12	6	0.57
(2,200)	1:18:B:MET:HB2	1:82:B:GLY:HA2	8	0.57
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	9	0.57
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD21	2	0.57
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	1	0.57
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD12	2	0.57
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	8	0.57
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	10	0.57
(1,969)	1:14:B:TRP:HZ3	1:62:B:GLN:HG3	5	0.57
(1,841)	1:54:B:ILE:HD13	1:23:B:PRO:HB3	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD1	1	0.57
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	9	0.57
(1,598)	1:26:B:ILE:HG21	1:90:B:GLY:HA3	1	0.57
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	10	0.57
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	7	0.57
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	1	0.57
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	2	0.57
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	1	0.57
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD11	10	0.57
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	1	0.57
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	9	0.57
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	1	0.57
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	4	0.57
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	8	0.57
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	5	0.57
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	8	0.57
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	10	0.57
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG23	4	0.56
(2,1524)	1:56:B:GLU:H	1:89:B:ILE:HG12	10	0.56
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	9	0.56
(2,1386)	1:64:B:GLU:H	1:15:B:LEU:HD23	1	0.56
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	10	0.56
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG21	3	0.56
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	2	0.56
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD21	6	0.56
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD21	10	0.56
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	1	0.56
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG23	8	0.56
(2,1157)	1:73:B:ILE:HG23	1:14:B:TRP:HZ3	3	0.56
(2,1157)	1:73:B:ILE:HG23	1:14:B:TRP:HZ3	5	0.56
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB3	3	0.56
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG21	3	0.56
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	3	0.56
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	5	0.56
(2,1078)	1:65:B:LEU:HD11	1:88:B:CYS:H	5	0.56
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	9	0.56
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG22	1	0.56
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	9	0.56
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	3	0.56
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	2	0.56
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	6	0.56
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE1	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE2	2	0.56
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE2	9	0.56
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	4	0.56
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	5	0.56
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD13	10	0.56
(2,874)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	7	0.56
(2,801)	1:89:B:ILE:HD11	1:86:B:GLY:HA3	3	0.56
(2,664)	1:57:B:SER:H	1:58:B:THR:HG21	6	0.56
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	3	0.56
(2,634)	1:98:B:LEU:HD12	1:93:B:PHE:HE1	4	0.56
(2,534)	1:96:B:LYS:HG2	1:96:B:LYS:HE2	8	0.56
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	1	0.56
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD1	9	0.56
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD13	1	0.56
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD21	7	0.56
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	5	0.56
(2,322)	1:76:B:GLU:HB3	1:75:B:SER:H	6	0.56
(2,131)	1:40:B:PHE:HB2	1:45:B:MET:HE1	10	0.56
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG21	5	0.56
(1,677)	1:5:B:ASN:HA	1:6:B:PRO:HD2	3	0.56
(1,677)	1:5:B:ASN:HA	1:6:B:PRO:HD2	7	0.56
(1,598)	1:26:B:ILE:HG21	1:90:B:GLY:HA3	2	0.56
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	10	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	3	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	5	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	6	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	7	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	9	0.56
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	10	0.56
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	2	0.56
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	5	0.56
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	9	0.56
(1,137)	1:41:B:ASP:H	1:40:B:PHE:HB2	9	0.56
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	10	0.55
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG23	7	0.55
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG21	10	0.55
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE3	7	0.55
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	5	0.55
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	10	0.55
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	7	0.55
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	1	0.55
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG23	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB3	7	0.55
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	9	0.55
(2,1103)	1:36:B:LEU:HD11	1:35:B:ASP:HB2	3	0.55
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	7	0.55
(2,1078)	1:65:B:LEU:HD13	1:88:B:CYS:H	2	0.55
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	4	0.55
(2,1000)	1:53:B:LEU:H	1:51:B:VAL:HB	8	0.55
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE3	4	0.55
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	10	0.55
(2,928)	1:65:B:LEU:HB3	1:15:B:LEU:HD21	9	0.55
(2,822)	1:73:B:ILE:HG23	1:75:B:SER:HA	6	0.55
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG22	7	0.55
(2,772)	1:13:B:ALA:HB3	1:16:B:ASN:HB3	5	0.55
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	3	0.55
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	4	0.55
(2,630)	1:15:B:LEU:HD11	1:15:B:LEU:HA	7	0.55
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	9	0.55
(2,520)	1:85:B:LEU:H	1:85:B:LEU:HD12	6	0.55
(2,495)	1:39:B:ARG:HG3	1:39:B:ARG:H	1	0.55
(2,480)	1:85:B:LEU:HG	1:89:B:ILE:H	6	0.55
(2,459)	1:34:B:PRO:HG2	1:34:B:PRO:HA	10	0.55
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	2	0.55
(2,282)	1:18:B:MET:HG2	1:85:B:LEU:HD23	8	0.55
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	3	0.55
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD22	10	0.55
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	10	0.55
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	6	0.55
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB3	9	0.55
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	6	0.55
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	6	0.55
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	7	0.55
(1,841)	1:54:B:ILE:HD13	1:23:B:PRO:HB3	2	0.55
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	6	0.55
(1,672)	1:21:B:LEU:H	1:20:B:PRO:HD3	4	0.55
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	2	0.55
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	6	0.55
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	8	0.55
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	3	0.55
(1,262)	1:11:B:LYS:H	1:11:B:LYS:HB2	2	0.55
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	10	0.55
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG13	6	0.55
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD21	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD13	2	0.54
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD12	9	0.54
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG22	1	0.54
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG22	2	0.54
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD11	6	0.54
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	5	0.54
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE3	8	0.54
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	9	0.54
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD13	2	0.54
(2,1359)	1:58:B:THR:H	1:54:B:ILE:HG13	7	0.54
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE2	1	0.54
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE2	4	0.54
(2,1268)	1:54:B:ILE:H	1:54:B:ILE:HG21	9	0.54
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	2	0.54
(2,1165)	1:54:B:ILE:HD13	1:50:B:CYS:HB2	9	0.54
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	10	0.54
(2,1023)	1:89:B:ILE:HG13	1:61:B:CYS:HA	5	0.54
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	7	0.54
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	7	0.54
(2,985)	1:62:B:GLN:HG3	1:59:B:LYS:HD3	2	0.54
(2,956)	1:50:B:CYS:HB2	1:93:B:PHE:HE1	6	0.54
(2,956)	1:40:B:PHE:HB3	1:40:B:PHE:HE1	7	0.54
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	1	0.54
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	2	0.54
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	3	0.54
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	9	0.54
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD11	3	0.54
(2,888)	1:73:B:ILE:H	1:73:B:ILE:HD11	1	0.54
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	8	0.54
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG23	10	0.54
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG23	4	0.54
(2,801)	1:89:B:ILE:HD12	1:86:B:GLY:HA3	7	0.54
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	2	0.54
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	8	0.54
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	7	0.54
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	1	0.54
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	10	0.54
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG22	10	0.54
(2,187)	1:97:B:HIS:HB3	1:98:B:LEU:HG	1	0.54
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	2	0.54
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD23	9	0.54
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG21	7	0.54
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	8	0.54
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD12	3	0.54
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	7	0.54
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	8	0.54
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	3	0.54
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	5	0.54
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB3	2	0.54
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	8	0.54
(1,982)	1:91:B:LYS:H	1:91:B:LYS:HG3	5	0.54
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	1	0.54
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD1	10	0.54
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	5	0.54
(1,690)	1:26:B:ILE:HD11	1:30:B:PHE:HE1	4	0.54
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	6	0.54
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	2	0.54
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	4	0.54
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	9	0.54
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	10	0.54
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	1	0.54
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	9	0.54
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	5	0.54
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG13	9	0.54
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG22	5	0.53
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG22	7	0.53
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG22	9	0.53
(2,1336)	1:94:B:ALA:H	1:98:B:LEU:HD22	4	0.53
(2,1114)	1:49:B:GLN:H	1:52:B:THR:HG21	1	0.53
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	4	0.53
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	5	0.53
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	5	0.53
(2,1058)	1:44:B:LYS:HD3	1:41:B:ASP:HB3	8	0.53
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	2	0.53
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	3	0.53
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	5	0.53
(2,1000)	1:30:B:PHE:H	1:28:B:LYS:HB3	10	0.53
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	3	0.53
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	8	0.53
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	7	0.53
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD3	7	0.53
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	5	0.53
(2,909)	1:99:B:ILE:HD12	1:95:B:GLU:HG2	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,908)	1:99:B:ILE:H	1:99:B:ILE:HD13	2	0.53
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD11	9	0.53
(2,896)	1:73:B:ILE:HD11	1:69:B:MET:HA	7	0.53
(2,890)	1:11:B:LYS:H	1:69:B:MET:HE3	9	0.53
(2,859)	1:51:B:VAL:HG11	1:23:B:PRO:HD2	5	0.53
(2,845)	1:100:B:PRO:HD3	1:43:B:ILE:HG13	10	0.53
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	10	0.53
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG21	5	0.53
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG23	6	0.53
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	9	0.53
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE1	7	0.53
(2,565)	1:15:B:LEU:HD21	1:62:B:GLN:HA	5	0.53
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	10	0.53
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	9	0.53
(2,545)	1:17:B:SER:HB3	1:14:B:TRP:HD1	7	0.53
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	6	0.53
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	2	0.53
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	9	0.53
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	10	0.53
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE2	2	0.53
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	5	0.53
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD3	3	0.53
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	10	0.53
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	9	0.53
(2,101)	1:74:B:ASN:HB2	1:75:B:SER:HA	3	0.53
(2,91)	1:90:B:GLY:H	1:93:B:PHE:HB3	3	0.53
(2,47)	1:87:B:GLU:H	1:85:B:LEU:HB3	6	0.53
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD13	6	0.53
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB2	7	0.53
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	8	0.53
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	7	0.53
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD12	8	0.53
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG21	8	0.53
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	3	0.53
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	2	0.53
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	1	0.53
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	3	0.53
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	5	0.53
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	7	0.53
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	10	0.53
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	1	0.53
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	8	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1580)	1:24:B:ASP:H	1:25:B:LEU:HB2	4	0.52
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	10	0.52
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD13	8	0.52
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG21	1	0.52
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG23	6	0.52
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE2	7	0.52
(2,1313)	1:66:B:TYR:H	1:66:B:TYR:HD2	9	0.52
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	7	0.52
(2,1211)	1:33:B:ASP:H	1:36:B:LEU:HD21	7	0.52
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	8	0.52
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	5	0.52
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	3	0.52
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	4	0.52
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	7	0.52
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	2	0.52
(2,1000)	1:53:B:LEU:H	1:51:B:VAL:HB	9	0.52
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	2	0.52
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	10	0.52
(2,909)	1:99:B:ILE:HD13	1:95:B:GLU:HG2	9	0.52
(2,896)	1:73:B:ILE:HD11	1:69:B:MET:HA	4	0.52
(2,822)	1:73:B:ILE:HG23	1:75:B:SER:HA	10	0.52
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG21	1	0.52
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE2	2	0.52
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE2	8	0.52
(2,772)	1:13:B:ALA:HB2	1:16:B:ASN:HB3	2	0.52
(2,772)	1:67:B:ALA:HB3	1:66:B:TYR:HB3	6	0.52
(2,772)	1:13:B:ALA:HB1	1:16:B:ASN:HB3	9	0.52
(2,762)	1:13:B:ALA:HB1	1:14:B:TRP:HB2	10	0.52
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	1	0.52
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	3	0.52
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	6	0.52
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	4	0.52
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	6	0.52
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	4	0.52
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	9	0.52
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	1	0.52
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	8	0.52
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	8	0.52
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	2	0.52
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	5	0.52
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	6	0.52
(1,1229)	1:96:B:LYS:H	1:98:B:LEU:HB3	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB3	5	0.52
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	4	0.52
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	6	0.52
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	7	0.52
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	8	0.52
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	7	0.52
(1,185)	1:101:B:LYS:H	1:101:B:LYS:HB3	1	0.52
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	1	0.52
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	4	0.52
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	6	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD23	2	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD23	7	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD21	9	0.52
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	10	0.52
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	5	0.51
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD21	6	0.51
(2,1538)	1:72:B:LYS:H	1:70:B:PRO:HG3	3	0.51
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD13	8	0.51
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD12	10	0.51
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	7	0.51
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	6	0.51
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	9	0.51
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG21	2	0.51
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG22	8	0.51
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG23	10	0.51
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG23	1	0.51
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE1	2	0.51
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	5	0.51
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE3	6	0.51
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	4	0.51
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG22	9	0.51
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	4	0.51
(2,934)	1:24:B:ASP:HB3	1:25:B:LEU:HB3	8	0.51
(2,921)	1:84:B:SER:HB3	1:81:B:TRP:HZ3	3	0.51
(2,906)	1:99:B:ILE:HD12	1:99:B:ILE:HB	7	0.51
(2,906)	1:99:B:ILE:HD13	1:99:B:ILE:HB	8	0.51
(2,906)	1:99:B:ILE:HD12	1:99:B:ILE:HB	9	0.51
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE3	7	0.51
(2,801)	1:89:B:ILE:HD13	1:86:B:GLY:HA3	9	0.51
(2,778)	1:31:B:ILE:HG21	1:32:B:GLN:HG3	2	0.51
(2,778)	1:31:B:ILE:HG22	1:32:B:GLN:HG3	4	0.51
(2,715)	1:51:B:VAL:HG12	1:27:B:CYS:HB3	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG23	1	0.51
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	10	0.51
(2,630)	1:15:B:LEU:HD13	1:15:B:LEU:HA	8	0.51
(2,606)	1:85:B:LEU:HD21	1:66:B:TYR:H	2	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	2	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	4	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	7	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	8	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	9	0.51
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	10	0.51
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE1	9	0.51
(2,526)	1:12:B:ASP:H	1:73:B:ILE:HG12	7	0.51
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	6	0.51
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD21	5	0.51
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	5	0.51
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HA	1	0.51
(2,104)	1:30:B:PHE:HB3	1:40:B:PHE:HE2	1	0.51
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	8	0.51
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	6	0.51
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	2	0.51
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	2	0.51
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG21	6	0.51
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	5	0.51
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	6	0.51
(1,307)	1:48:B:GLU:H	1:48:B:GLU:HB3	6	0.51
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD23	2	0.51
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD21	7	0.51
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	7	0.51
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	9	0.51
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD21	3	0.51
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD23	4	0.51
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD23	5	0.51
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	6	0.51
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	6	0.5
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	4	0.5
(2,1523)	1:56:B:GLU:H	1:23:B:PRO:HG2	7	0.5
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	9	0.5
(2,1478)	1:27:B:CYS:H	1:54:B:ILE:HG22	2	0.5
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	1	0.5
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	4	0.5
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	1	0.5
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1387)	1:64:B:GLU:H	1:65:B:LEU:HD12	3	0.5
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	6	0.5
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	9	0.5
(2,1123)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	8	0.5
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD23	1	0.5
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	7	0.5
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	7	0.5
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	7	0.5
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	2	0.5
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	2	0.5
(2,1009)	1:66:B:TYR:HA	1:11:B:LYS:HB3	10	0.5
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB3	5	0.5
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	1	0.5
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	3	0.5
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	1	0.5
(2,956)	1:50:B:CYS:HB2	1:47:B:TYR:HD1	10	0.5
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	8	0.5
(2,925)	1:83:B:ARG:H	1:83:B:ARG:HD2	2	0.5
(2,906)	1:99:B:ILE:HD11	1:99:B:ILE:HB	4	0.5
(2,906)	1:99:B:ILE:HD13	1:99:B:ILE:HB	10	0.5
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD13	1	0.5
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	1	0.5
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG23	4	0.5
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG21	4	0.5
(2,772)	1:13:B:ALA:HB1	1:16:B:ASN:HB3	8	0.5
(2,772)	1:13:B:ALA:HB3	1:16:B:ASN:HB3	10	0.5
(2,601)	1:72:B:LYS:HB3	1:72:B:LYS:HG3	5	0.5
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	8	0.5
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	8	0.5
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	3	0.5
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	8	0.5
(2,409)	1:97:B:HIS:HB3	1:96:B:LYS:HD3	7	0.5
(2,360)	1:22:B:LEU:H	1:23:B:PRO:HG3	9	0.5
(2,150)	1:64:B:GLU:H	1:64:B:GLU:HG2	3	0.5
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG23	7	0.5
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	2	0.5
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	7	0.5
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB1	4	0.5
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB1	8	0.5
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	5	0.5
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG21	9	0.5
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:5:B:ASN:HA	1:6:B:PRO:HD2	1	0.5
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	4	0.5
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	6	0.5
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	9	0.5
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	2	0.5
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	3	0.5
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	8	0.5
(1,44)	1:98:B:LEU:HB2	1:98:B:LEU:HD22	8	0.5
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	3	0.5
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG23	3	0.49
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	1	0.49
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB3	8	0.49
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	3	0.49
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG21	6	0.49
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	6	0.49
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	8	0.49
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	4	0.49
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	4	0.49
(2,1028)	1:43:B:ILE:H	1:44:B:LYS:HD2	3	0.49
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG22	4	0.49
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	5	0.49
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	7	0.49
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	2	0.49
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	6	0.49
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	3	0.49
(2,961)	1:50:B:CYS:HB3	1:54:B:ILE:HG12	3	0.49
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	4	0.49
(2,948)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	3	0.49
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	4	0.49
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	8	0.49
(2,932)	1:60:B:LYS:HE3	1:60:B:LYS:HB2	3	0.49
(2,890)	1:11:B:LYS:H	1:69:B:MET:HE3	10	0.49
(2,889)	1:73:B:ILE:HD13	1:78:B:ALA:H	4	0.49
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE1	10	0.49
(2,859)	1:51:B:VAL:HG11	1:23:B:PRO:HD2	3	0.49
(2,694)	1:42:B:GLU:HA	1:42:B:GLU:HG3	4	0.49
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	8	0.49
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	9	0.49
(2,634)	1:98:B:LEU:HD13	1:93:B:PHE:HE1	3	0.49
(2,606)	1:85:B:LEU:HD21	1:66:B:TYR:H	1	0.49
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	4	0.49
(2,444)	1:20:B:PRO:HG2	1:21:B:LEU:HD11	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	2	0.49
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	10	0.49
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	7	0.49
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	8	0.49
(2,341)	1:38:B:LYS:HD2	1:38:B:LYS:HA	6	0.49
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	4	0.49
(2,46)	1:61:B:CYS:HB3	1:89:B:ILE:HD13	1	0.49
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	1	0.49
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	5	0.49
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	9	0.49
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG23	10	0.49
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	5	0.49
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	7	0.49
(1,921)	1:85:B:LEU:H	1:84:B:SER:HB2	10	0.49
(1,827)	1:89:B:ILE:HG22	1:93:B:PHE:HD2	4	0.49
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	7	0.49
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	2	0.49
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	9	0.49
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD13	6	0.49
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	1	0.49
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	10	0.49
(1,88)	1:30:B:PHE:H	1:30:B:PHE:HB3	5	0.49
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	6	0.49
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	7	0.48
(2,1553)	1:96:B:LYS:H	1:96:B:LYS:HE3	6	0.48
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD11	2	0.48
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	6	0.48
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD12	4	0.48
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD13	4	0.48
(2,1313)	1:66:B:TYR:H	1:69:B:MET:H	10	0.48
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD11	4	0.48
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	7	0.48
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	5	0.48
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD21	7	0.48
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD23	1	0.48
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD21	7	0.48
(2,1091)	1:14:B:TRP:HA	1:9:B:MET:HE1	6	0.48
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	2	0.48
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	10	0.48
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	6	0.48
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG21	6	0.48
(2,1029)	1:44:B:LYS:HD2	1:43:B:ILE:HA	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	6	0.48
(2,1016)	1:64:B:GLU:HB3	1:65:B:LEU:HB3	7	0.48
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	5	0.48
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	5	0.48
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	8	0.48
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	9	0.48
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	5	0.48
(2,959)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	10	0.48
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	7	0.48
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	2	0.48
(2,889)	1:73:B:ILE:HD13	1:78:B:ALA:H	7	0.48
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	1	0.48
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	8	0.48
(2,845)	1:100:B:PRO:HD3	1:43:B:ILE:HG13	5	0.48
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	3	0.48
(2,694)	1:42:B:GLU:HA	1:42:B:GLU:HG3	5	0.48
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	9	0.48
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	7	0.48
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	1	0.48
(2,430)	1:23:B:PRO:HG2	1:54:B:ILE:HG21	2	0.48
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	1	0.48
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	3	0.48
(2,303)	1:61:B:CYS:H	1:60:B:LYS:HD3	3	0.48
(2,268)	1:45:B:MET:HG2	1:98:B:LEU:HD23	1	0.48
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD2	8	0.48
(2,216)	1:8:B:GLU:HB2	1:74:B:ASN:HB2	5	0.48
(2,188)	1:0:B:MET:HB3	1:-1:B:LYS:H	1	0.48
(2,154)	1:56:B:GLU:HG3	1:53:B:LEU:HB3	1	0.48
(2,131)	1:40:B:PHE:HB2	1:45:B:MET:HE2	6	0.48
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG2	7	0.48
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	9	0.48
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG22	7	0.48
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	10	0.48
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	7	0.48
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	9	0.48
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	8	0.48
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	1	0.48
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	3	0.48
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	4	0.48
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	5	0.48
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	9	0.48
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:54:B:ILE:HD12	1:89:B:ILE:HG22	8	0.48
(1,841)	1:54:B:ILE:HD11	1:23:B:PRO:HB3	4	0.48
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	10	0.48
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	4	0.48
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	6	0.48
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	10	0.48
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	4	0.48
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	8	0.48
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	10	0.48
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	8	0.48
(1,269)	1:18:B:MET:HG3	1:18:B:MET:HA	8	0.48
(1,252)	1:45:B:MET:HB2	1:40:B:PHE:HA	1	0.48
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	2	0.48
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	6	0.48
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	1	0.48
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	3	0.48
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG13	4	0.48
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	2	0.47
(2,1567)	1:71:B:ASP:H	1:11:B:LYS:HD3	5	0.47
(2,1446)	1:57:B:SER:H	1:56:B:GLU:HB3	6	0.47
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG22	2	0.47
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD13	10	0.47
(2,1346)	1:99:B:ILE:H	1:99:B:ILE:HG21	4	0.47
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB2	4	0.47
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB1	5	0.47
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB3	10	0.47
(2,1099)	1:22:B:LEU:H	1:22:B:LEU:HD13	5	0.47
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE1	7	0.47
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	2	0.47
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	2	0.47
(2,1066)	1:43:B:ILE:HG13	1:44:B:LYS:H	6	0.47
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	7	0.47
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	8	0.47
(2,1001)	1:8:B:GLU:HB3	1:73:B:ILE:H	9	0.47
(2,943)	1:27:B:CYS:HB3	1:28:B:LYS:HD3	8	0.47
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	10	0.47
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	4	0.47
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	5	0.47
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	6	0.47
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	7	0.47
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	8	0.47
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG22	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG21	9	0.47
(2,802)	1:26:B:ILE:HG21	1:86:B:GLY:HA2	1	0.47
(2,778)	1:99:B:ILE:HG23	1:95:B:GLU:HG2	5	0.47
(2,772)	1:13:B:ALA:HB2	1:16:B:ASN:HB3	1	0.47
(2,772)	1:13:B:ALA:HB1	1:16:B:ASN:HB3	4	0.47
(2,687)	1:38:B:LYS:HA	1:41:B:ASP:H	2	0.47
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	4	0.47
(2,528)	1:22:B:LEU:HD23	1:86:B:GLY:HA3	8	0.47
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	2	0.47
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	6	0.47
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD3	6	0.47
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	6	0.47
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	10	0.47
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	1	0.47
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	6	0.47
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	2	0.47
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG22	5	0.47
(2,221)	1:69:B:MET:HB2	1:11:B:LYS:HA	7	0.47
(2,119)	1:47:B:TYR:HB2	1:46:B:THR:HB	7	0.47
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD13	5	0.47
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	10	0.47
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD11	10	0.47
(2,46)	1:92:B:ASP:HB3	1:89:B:ILE:HG23	8	0.47
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	7	0.47
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD11	9	0.47
(2,16)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	9	0.47
(2,8)	1:35:B:ASP:H	1:33:B:ASP:HB2	7	0.47
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	10	0.47
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB1	8	0.47
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG22	1	0.47
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	10	0.47
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB3	3	0.47
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	1	0.47
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD11	5	0.47
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	1	0.47
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	3	0.47
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	10	0.47
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	2	0.47
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	1	0.47
(1,447)	1:60:B:LYS:HG3	1:61:B:CYS:HA	2	0.47
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD12	5	0.47
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD22	3	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD22	5	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD22	6	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD23	9	0.47
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD21	10	0.47
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	1	0.47
(1,188)	1:96:B:LYS:H	1:96:B:LYS:HB3	3	0.47
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	5	0.47
(1,33)	1:24:B:ASP:HB2	1:51:B:VAL:HG12	7	0.47
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	6	0.46
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	8	0.46
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	9	0.46
(2,1580)	1:24:B:ASP:H	1:25:B:LEU:HB2	9	0.46
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD11	4	0.46
(2,1495)	1:25:B:LEU:H	1:26:B:ILE:HG21	7	0.46
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE3	6	0.46
(2,1391)	1:88:B:CYS:H	1:89:B:ILE:HD13	5	0.46
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	7	0.46
(2,1362)	1:11:B:LYS:H	1:11:B:LYS:HB2	8	0.46
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	1	0.46
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD12	1	0.46
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	9	0.46
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	1	0.46
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB2	9	0.46
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	1	0.46
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	8	0.46
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	3	0.46
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	4	0.46
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	3	0.46
(2,956)	1:50:B:CYS:HB2	1:40:B:PHE:HE2	4	0.46
(2,905)	1:28:B:LYS:HG3	1:31:B:ILE:HD12	1	0.46
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	4	0.46
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	1	0.46
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	2	0.46
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	10	0.46
(2,762)	1:13:B:ALA:HB3	1:14:B:TRP:HB2	1	0.46
(2,762)	1:13:B:ALA:HB1	1:14:B:TRP:HB2	5	0.46
(2,661)	1:73:B:ILE:H	1:10:B:THR:HG22	7	0.46
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG23	5	0.46
(2,628)	1:65:B:LEU:HD22	1:68:B:SER:HB2	7	0.46
(2,606)	1:85:B:LEU:HD23	1:66:B:TYR:H	9	0.46
(2,606)	1:85:B:LEU:HD22	1:66:B:TYR:H	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HD2	10	0.46
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	5	0.46
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	7	0.46
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	6	0.46
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	10	0.46
(2,262)	1:60:B:LYS:HD2	1:60:B:LYS:HA	10	0.46
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG22	8	0.46
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD3	1	0.46
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	9	0.46
(2,36)	1:37:B:LYS:HE3	1:31:B:ILE:HA	1	0.46
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	10	0.46
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	4	0.46
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG21	6	0.46
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	5	0.46
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	6	0.46
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	9	0.46
(1,841)	1:54:B:ILE:HD12	1:23:B:PRO:HB3	8	0.46
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB2	7	0.46
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB3	7	0.46
(1,827)	1:89:B:ILE:HG21	1:93:B:PHE:HD1	6	0.46
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	3	0.46
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG22	10	0.46
(1,812)	1:80:B:THR:HG21	1:81:B:TRP:HZ2	10	0.46
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	9	0.46
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE2	4	0.46
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	5	0.46
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	7	0.46
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	2	0.46
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD23	8	0.46
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	9	0.46
(1,120)	1:48:B:GLU:H	1:47:B:TYR:HB2	7	0.46
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	9	0.46
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	3	0.45
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	10	0.45
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG23	6	0.45
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	1	0.45
(2,1362)	1:11:B:LYS:H	1:11:B:LYS:HB2	3	0.45
(2,1362)	1:11:B:LYS:H	1:11:B:LYS:HB2	9	0.45
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	2	0.45
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	9	0.45
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE2	6	0.45
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	8	0.45
(2,1180)	1:68:B:SER:HB2	1:67:B:ALA:HB3	9	0.45
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG23	8	0.45
(2,1113)	1:49:B:GLN:H	1:52:B:THR:HG21	1	0.45
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG23	9	0.45
(2,1099)	1:22:B:LEU:H	1:22:B:LEU:HD12	2	0.45
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD23	6	0.45
(2,1097)	1:98:B:LEU:HD21	1:39:B:ARG:HA	2	0.45
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE1	6	0.45
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	3	0.45
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	7	0.45
(2,1084)	1:53:B:LEU:HD11	1:96:B:LYS:HD3	3	0.45
(2,1078)	1:65:B:LEU:HD11	1:88:B:CYS:H	8	0.45
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	5	0.45
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG21	4	0.45
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	8	0.45
(2,1043)	1:33:B:ASP:H	1:37:B:LYS:HD3	3	0.45
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	5	0.45
(2,1009)	1:73:B:ILE:HA	1:11:B:LYS:HB3	1	0.45
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG2	6	0.45
(2,1000)	1:53:B:LEU:H	1:51:B:VAL:HB	5	0.45
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	8	0.45
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	10	0.45
(2,988)	1:59:B:LYS:HB2	1:55:B:PRO:HB3	8	0.45
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	5	0.45
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	8	0.45
(2,956)	1:50:B:CYS:HB2	1:40:B:PHE:HE1	8	0.45
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	3	0.45
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	6	0.45
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	9	0.45
(2,839)	1:20:B:PRO:HB2	1:20:B:PRO:HD2	9	0.45
(2,822)	1:73:B:ILE:HG21	1:75:B:SER:HA	9	0.45
(2,801)	1:89:B:ILE:HD11	1:86:B:GLY:HA3	2	0.45
(2,762)	1:13:B:ALA:HB3	1:14:B:TRP:HB2	2	0.45
(2,584)	1:67:B:ALA:H	1:66:B:TYR:HA	10	0.45
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	8	0.45
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	2	0.45
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE2	3	0.45
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	5	0.45
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	6	0.45
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	9	0.45
(2,405)	1:31:B:ILE:HG13	1:30:B:PHE:HB3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG13	1	0.45
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	4	0.45
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE1	9	0.45
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	6	0.45
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	1	0.45
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	6	0.45
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	9	0.45
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	9	0.45
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	5	0.45
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	8	0.45
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	4	0.45
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB3	3	0.45
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG22	2	0.45
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	8	0.45
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD1	8	0.45
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	9	0.45
(1,718)	1:90:B:GLY:HA3	1:94:B:ALA:H	5	0.45
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	6	0.45
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	4	0.45
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	3	0.45
(1,294)	1:48:B:GLU:HB3	1:46:B:THR:HB	6	0.45
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	4	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	1	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	2	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	3	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	4	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	6	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	7	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	8	0.45
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	10	0.45
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	2	0.45
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	2	0.44
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	10	0.44
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	10	0.44
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	2	0.44
(2,1535)	1:72:B:LYS:H	1:72:B:LYS:HE3	6	0.44
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD11	3	0.44
(2,1465)	1:22:B:LEU:H	1:21:B:LEU:HD12	7	0.44
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB1	2	0.44
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB2	6	0.44
(2,1442)	1:8:B:GLU:H	1:72:B:LYS:HD3	1	0.44
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	3	0.44
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	10	0.44
(2,1362)	1:11:B:LYS:H	1:11:B:LYS:HB2	2	0.44
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	7	0.44
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	7	0.44
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD13	1	0.44
(2,1276)	1:62:B:GLN:H	1:89:B:ILE:HD11	5	0.44
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	2	0.44
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD12	2	0.44
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	7	0.44
(2,1117)	1:-6:B:VAL:HG21	1:-4:B:ASP:H	8	0.44
(2,1107)	1:54:B:ILE:HG12	1:27:B:CYS:HA	3	0.44
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD21	3	0.44
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	10	0.44
(2,1078)	1:65:B:LEU:HD11	1:88:B:CYS:H	10	0.44
(2,1065)	1:100:B:PRO:HG2	1:101:B:LYS:HD2	4	0.44
(2,1058)	1:44:B:LYS:HD2	1:41:B:ASP:HB3	4	0.44
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	5	0.44
(2,989)	1:69:B:MET:HB2	1:70:B:PRO:HA	9	0.44
(2,985)	1:62:B:GLN:HG3	1:59:B:LYS:HD3	1	0.44
(2,939)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	8	0.44
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE3	3	0.44
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG22	2	0.44
(2,762)	1:13:B:ALA:HB2	1:14:B:TRP:HB2	4	0.44
(2,627)	1:65:B:LEU:HD22	1:85:B:LEU:H	6	0.44
(2,608)	1:85:B:LEU:HD22	1:62:B:GLN:HB2	7	0.44
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	1	0.44
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE1	2	0.44
(2,566)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	6	0.44
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	3	0.44
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	5	0.44
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	7	0.44
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	7	0.44
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	9	0.44
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	4	0.44
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD21	3	0.44
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	2	0.44
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	2	0.44
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	4	0.44
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	4	0.44
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	4	0.44
(2,170)	1:62:B:GLN:HG3	1:85:B:LEU:HD23	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	7	0.44
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	10	0.44
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	1	0.44
(1,1349)	1:15:B:LEU:H	1:11:B:LYS:HB3	2	0.44
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	2	0.44
(1,844)	1:54:B:ILE:HD11	1:89:B:ILE:HG23	4	0.44
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	8	0.44
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	2	0.44
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	4	0.44
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	2	0.44
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	3	0.44
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	9	0.44
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD11	5	0.44
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	4	0.44
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	3	0.44
(1,24)	1:36:B:LEU:H	1:33:B:ASP:HB2	7	0.44
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	6	0.43
(2,1580)	1:24:B:ASP:H	1:25:B:LEU:HB2	8	0.43
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	10	0.43
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	7	0.43
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	1	0.43
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	10	0.43
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG21	4	0.43
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	6	0.43
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD13	5	0.43
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB3	5	0.43
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	0.43
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB2	2	0.43
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB1	6	0.43
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB1	9	0.43
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	9	0.43
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG23	8	0.43
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD23	8	0.43
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	5	0.43
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	2	0.43
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	8	0.43
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	10	0.43
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	8	0.43
(2,1000)	1:53:B:LEU:H	1:51:B:VAL:HB	3	0.43
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	5	0.43
(2,964)	1:16:B:ASN:HB2	1:15:B:LEU:HB3	9	0.43
(2,948)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,948)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	9	0.43
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	7	0.43
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD13	2	0.43
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE2	4	0.43
(2,859)	1:51:B:VAL:HG13	1:23:B:PRO:HD2	1	0.43
(2,859)	1:51:B:VAL:HG13	1:23:B:PRO:HD2	6	0.43
(2,829)	1:98:B:LEU:H	1:43:B:ILE:HG22	9	0.43
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	4	0.43
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG22	2	0.43
(2,778)	1:99:B:ILE:HG23	1:95:B:GLU:HG2	8	0.43
(2,761)	1:13:B:ALA:HB1	1:9:B:MET:HA	7	0.43
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	7	0.43
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD22	6	0.43
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE3	7	0.43
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	4	0.43
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	10	0.43
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	7	0.43
(2,409)	1:97:B:HIS:HB3	1:96:B:LYS:HD3	4	0.43
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	1	0.43
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE2	8	0.43
(2,370)	1:59:B:LYS:HD2	1:59:B:LYS:HA	10	0.43
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	3	0.43
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG11	5	0.43
(2,249)	1:100:B:PRO:HB3	1:43:B:ILE:HG21	1	0.43
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	2	0.43
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	9	0.43
(2,187)	1:97:B:HIS:HB3	1:43:B:ILE:HG13	2	0.43
(2,186)	1:97:B:HIS:H	1:97:B:HIS:HB3	2	0.43
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	5	0.43
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	7	0.43
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	8	0.43
(2,108)	1:30:B:PHE:HB2	1:98:B:LEU:HD12	8	0.43
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG22	6	0.43
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD13	5	0.43
(2,81)	1:12:B:ASP:HB2	1:15:B:LEU:HD11	8	0.43
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	3	0.43
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	4	0.43
(1,1093)	1:26:B:ILE:H	1:26:B:ILE:HG23	3	0.43
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	3	0.43
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD21	9	0.43
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	3	0.43
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB1	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:91:B:LYS:H	1:89:B:ILE:HG23	2	0.43
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	2	0.43
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	1	0.43
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	6	0.43
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	9	0.43
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	2	0.43
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	6	0.43
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	7	0.43
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	4	0.43
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	6	0.43
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	2	0.43
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	5	0.43
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	10	0.43
(1,194)	1:60:B:LYS:HB3	1:60:B:LYS:HA	5	0.43
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	2	0.43
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	7	0.42
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	9	0.42
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG23	9	0.42
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD12	7	0.42
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE1	8	0.42
(2,1157)	1:73:B:ILE:HG21	1:14:B:TRP:HZ3	4	0.42
(2,1156)	1:43:B:ILE:HD13	1:100:B:PRO:HG3	5	0.42
(2,1153)	1:27:B:CYS:H	1:54:B:ILE:HG22	10	0.42
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE1	8	0.42
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG22	5	0.42
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD21	9	0.42
(2,1088)	1:60:B:LYS:HG2	1:57:B:SER:HA	1	0.42
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	5	0.42
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	7	0.42
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	9	0.42
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	10	0.42
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	3	0.42
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	5	0.42
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	4	0.42
(2,934)	1:24:B:ASP:HB3	1:21:B:LEU:HB3	10	0.42
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD12	8	0.42
(2,894)	1:14:B:TRP:HB3	1:69:B:MET:HE1	1	0.42
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	8	0.42
(2,874)	1:26:B:ILE:HD11	1:90:B:GLY:HA3	6	0.42
(2,713)	1:51:B:VAL:HG22	1:52:B:THR:HB	10	0.42
(2,663)	1:70:B:PRO:HB2	1:77:B:THR:HG23	6	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	3	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	4	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	5	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	6	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	7	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	8	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	9	0.42
(2,600)	1:72:B:LYS:HG2	1:72:B:LYS:HB2	10	0.42
(2,566)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	5	0.42
(2,514)	1:22:B:LEU:HD21	1:82:B:GLY:HA3	6	0.42
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE2	1	0.42
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	5	0.42
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	10	0.42
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	3	0.42
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	5	0.42
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	6	0.42
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	1	0.42
(2,409)	1:97:B:HIS:HB3	1:96:B:LYS:HD3	9	0.42
(2,405)	1:31:B:ILE:HG13	1:30:B:PHE:HB3	5	0.42
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	1	0.42
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	9	0.42
(2,332)	1:55:B:PRO:HG3	1:51:B:VAL:HA	1	0.42
(2,332)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	5	0.42
(2,263)	1:19:B:THR:HB	1:20:B:PRO:HB3	8	0.42
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	4	0.42
(2,186)	1:97:B:HIS:H	1:97:B:HIS:HB3	3	0.42
(2,186)	1:98:B:LEU:H	1:97:B:HIS:HB3	5	0.42
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	2	0.42
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	7	0.42
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	3	0.42
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	1	0.42
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	4	0.42
(2,45)	1:61:B:CYS:HB3	1:65:B:LEU:HG	3	0.42
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	3	0.42
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	1	0.42
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	4	0.42
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	1	0.42
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	4	0.42
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	7	0.42
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	1	0.42
(1,913)	1:13:B:ALA:H	1:10:B:THR:HG23	4	0.42
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB3	2	0.42
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	7	0.42
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG22	2	0.42
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	4	0.42
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	10	0.42
(1,549)	1:25:B:LEU:HB3	1:25:B:LEU:HA	4	0.42
(1,549)	1:25:B:LEU:HB3	1:25:B:LEU:HA	8	0.42
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	6	0.42
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD13	8	0.42
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	9	0.42
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	2	0.42
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	8	0.42
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	9	0.41
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB3	7	0.41
(2,1381)	1:30:B:PHE:H	1:26:B:ILE:HB	8	0.41
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	4	0.41
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG21	5	0.41
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB1	8	0.41
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB3	10	0.41
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	4	0.41
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB1	3	0.41
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	8	0.41
(2,1117)	1:-6:B:VAL:HG22	1:-4:B:ASP:H	4	0.41
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	4	0.41
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	6	0.41
(2,1078)	1:65:B:LEU:HD13	1:88:B:CYS:H	1	0.41
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	3	0.41
(2,988)	1:-1:B:LYS:HB2	1:0:B:MET:HG3	5	0.41
(2,925)	1:83:B:ARG:H	1:83:B:ARG:HD2	9	0.41
(2,894)	1:14:B:TRP:HB3	1:69:B:MET:HE1	7	0.41
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	10	0.41
(2,885)	1:79:B:GLY:HA2	1:18:B:MET:HE3	10	0.41
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	2	0.41
(2,859)	1:51:B:VAL:HG12	1:23:B:PRO:HD2	7	0.41
(2,859)	1:51:B:VAL:HG13	1:23:B:PRO:HD2	10	0.41
(2,845)	1:100:B:PRO:HD3	1:43:B:ILE:HG13	3	0.41
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	1	0.41
(2,666)	1:22:B:LEU:HD12	1:22:B:LEU:HA	5	0.41
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD11	3	0.41
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD22	10	0.41
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	3	0.41
(2,391)	1:37:B:LYS:HD3	1:40:B:PHE:HE1	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,332)	1:55:B:PRO:HG3	1:51:B:VAL:HA	4	0.41
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	9	0.41
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD22	1	0.41
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD21	6	0.41
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	1	0.41
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	4	0.41
(2,146)	1:8:B:GLU:HG2	1:8:B:GLU:HA	6	0.41
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	5	0.41
(2,5)	1:65:B:LEU:HB2	1:85:B:LEU:HD12	7	0.41
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	5	0.41
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB2	1	0.41
(1,937)	1:73:B:ILE:H	1:72:B:LYS:HG3	10	0.41
(1,728)	1:26:B:ILE:HD12	1:86:B:GLY:HA3	8	0.41
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	1	0.41
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG22	1	0.41
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	6	0.41
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	9	0.41
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	10	0.41
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	5	0.41
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	1	0.41
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	6	0.41
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	7	0.41
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	1	0.41
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	6	0.41
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	2	0.4
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	7	0.4
(2,1553)	1:96:B:LYS:H	1:96:B:LYS:HE3	3	0.4
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	8	0.4
(2,1474)	1:63:B:ASP:H	1:60:B:LYS:HG3	2	0.4
(2,1424)	1:44:B:LYS:H	1:44:B:LYS:HE2	2	0.4
(2,1416)	1:41:B:ASP:H	1:45:B:MET:HE2	10	0.4
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG21	4	0.4
(2,1390)	1:88:B:CYS:H	1:87:B:GLU:HB3	3	0.4
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	9	0.4
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	6	0.4
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG23	2	0.4
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	4	0.4
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	9	0.4
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG23	9	0.4
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB2	6	0.4
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD23	4	0.4
(2,1095)	1:15:B:LEU:HD12	1:66:B:TYR:H	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD13	6	0.4
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	1	0.4
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	3	0.4
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	8	0.4
(2,1020)	1:92:B:ASP:HB2	1:60:B:LYS:HD3	9	0.4
(2,985)	1:32:B:GLN:HG2	1:28:B:LYS:HD3	3	0.4
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	6	0.4
(2,896)	1:73:B:ILE:HD13	1:69:B:MET:HA	9	0.4
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	10	0.4
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	3	0.4
(2,874)	1:26:B:ILE:HD11	1:90:B:GLY:HA3	8	0.4
(2,822)	1:73:B:ILE:HG21	1:75:B:SER:HA	1	0.4
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG22	3	0.4
(2,762)	1:13:B:ALA:HB2	1:14:B:TRP:HB2	8	0.4
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	6	0.4
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD1	10	0.4
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG23	4	0.4
(2,514)	1:22:B:LEU:HD23	1:82:B:GLY:HA3	10	0.4
(2,506)	1:28:B:LYS:HG3	1:25:B:LEU:HA	9	0.4
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	3	0.4
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	1	0.4
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	1	0.4
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG23	3	0.4
(2,171)	1:32:B:GLN:HG2	1:33:B:ASP:H	9	0.4
(2,164)	1:62:B:GLN:HG3	1:66:B:TYR:HD1	9	0.4
(2,148)	1:8:B:GLU:HG3	1:72:B:LYS:HB2	1	0.4
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	8	0.4
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG22	9	0.4
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG23	10	0.4
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	10	0.4
(1,1088)	1:49:B:GLN:H	1:48:B:GLU:HB3	3	0.4
(1,866)	1:101:B:LYS:H	1:101:B:LYS:HG3	6	0.4
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD12	6	0.4
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB1	6	0.4
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB1	10	0.4
(1,766)	1:99:B:ILE:HG23	1:101:B:LYS:HB3	6	0.4
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	3	0.4
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE1	3	0.4
(1,721)	1:90:B:GLY:HA3	1:93:B:PHE:HD1	2	0.4
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	1	0.4
(1,425)	1:91:B:LYS:HG2	1:91:B:LYS:HA	5	0.4
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	1	0.4
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	3	0.4
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	8	0.4
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	9	0.4
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	3	0.39
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	4	0.39
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	7	0.39
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD11	5	0.39
(2,1320)	1:40:B:PHE:H	1:38:B:LYS:HB3	6	0.39
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	8	0.39
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	9	0.39
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB1	2	0.39
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB1	3	0.39
(2,1165)	1:54:B:ILE:HD13	1:50:B:CYS:HB2	8	0.39
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HZ3	2	0.39
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB3	2	0.39
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG21	10	0.39
(2,1097)	1:98:B:LEU:HD21	1:39:B:ARG:HA	9	0.39
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	1	0.39
(2,1030)	1:44:B:LYS:HD2	1:41:B:ASP:HB2	1	0.39
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD2	9	0.39
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG3	9	0.39
(2,990)	1:89:B:ILE:HA	1:91:B:LYS:HB2	6	0.39
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD13	6	0.39
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD12	7	0.39
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD11	5	0.39
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	1	0.39
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	3	0.39
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	9	0.39
(2,810)	1:58:B:THR:H	1:54:B:ILE:HG21	8	0.39
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG22	9	0.39
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB3	3	0.39
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	5	0.39
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	6	0.39
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	8	0.39
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE2	3	0.39
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	9	0.39
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	7	0.39
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE1	4	0.39
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	4	0.39
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	9	0.39
(2,514)	1:22:B:LEU:HD23	1:82:B:GLY:HA3	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE2	8	0.39
(2,430)	1:37:B:LYS:HD2	1:31:B:ILE:HG21	6	0.39
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	4	0.39
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	2	0.39
(2,374)	1:23:B:PRO:HG2	1:55:B:PRO:HB3	6	0.39
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	3	0.39
(2,303)	1:61:B:CYS:H	1:60:B:LYS:HD3	9	0.39
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	6	0.39
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG21	4	0.39
(2,232)	1:28:B:LYS:HE3	1:28:B:LYS:HB2	10	0.39
(2,200)	1:69:B:MET:HB2	1:11:B:LYS:HA	7	0.39
(2,186)	1:97:B:HIS:H	1:97:B:HIS:HB3	1	0.39
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	2	0.39
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	2	0.39
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	3	0.39
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	9	0.39
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	1	0.39
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	9	0.39
(1,1121)	1:44:B:LYS:H	1:98:B:LEU:HD21	3	0.39
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	6	0.39
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	8	0.39
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB3	1	0.39
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB3	9	0.39
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB3	10	0.39
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	10	0.39
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	8	0.39
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	5	0.39
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	7	0.39
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	5	0.39
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	3	0.39
(1,391)	1:99:B:ILE:HG12	1:94:B:ALA:HB3	5	0.39
(1,365)	1:36:B:LEU:H	1:36:B:LEU:HG	5	0.39
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	7	0.39
(1,249)	1:52:B:THR:HB	1:53:B:LEU:HD22	1	0.39
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD22	4	0.38
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	9	0.38
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	5	0.38
(2,1535)	1:72:B:LYS:H	1:72:B:LYS:HE3	3	0.38
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD13	1	0.38
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD12	3	0.38
(2,1456)	1:93:B:PHE:H	1:54:B:ILE:HG22	4	0.38
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1358)	1:58:B:THR:H	1:59:B:LYS:HB2	8	0.38
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD12	6	0.38
(2,1324)	1:40:B:PHE:H	1:98:B:LEU:HD12	10	0.38
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD13	7	0.38
(2,1144)	1:17:B:SER:HB2	1:9:B:MET:HE1	2	0.38
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	10	0.38
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB3	6	0.38
(2,985)	1:32:B:GLN:HG2	1:28:B:LYS:HD2	8	0.38
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	2	0.38
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	10	0.38
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD12	4	0.38
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD11	4	0.38
(2,889)	1:73:B:ILE:HD13	1:78:B:ALA:H	5	0.38
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	7	0.38
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	7	0.38
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	9	0.38
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	2	0.38
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	4	0.38
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	5	0.38
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	7	0.38
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	10	0.38
(2,789)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	3	0.38
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG22	10	0.38
(2,772)	1:13:B:ALA:HB3	1:16:B:ASN:HB3	7	0.38
(2,596)	1:61:B:CYS:H	1:60:B:LYS:HG3	1	0.38
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	7	0.38
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	8	0.38
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	7	0.38
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	8	0.38
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	4	0.38
(2,392)	1:49:B:GLN:HB3	1:47:B:TYR:H	7	0.38
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	3	0.38
(2,245)	1:6:B:PRO:HB2	1:6:B:PRO:HD3	5	0.38
(2,96)	1:93:B:PHE:HB3	1:98:B:LEU:HD11	1	0.38
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	2	0.38
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	3	0.38
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB1	6	0.38
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	9	0.38
(1,1022)	1:40:B:PHE:H	1:45:B:MET:HB2	1	0.38
(1,822)	1:70:B:PRO:HG3	1:73:B:ILE:HA	1	0.38
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	3	0.38
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	7	0.38
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	8	0.38
(1,615)	1:43:B:ILE:HD13	1:98:B:LEU:HA	1	0.38
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	8	0.38
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	10	0.38
(1,485)	1:98:B:LEU:HD21	1:40:B:PHE:HB3	4	0.38
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	1	0.38
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	5	0.38
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD13	3	0.38
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	1	0.37
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD23	5	0.37
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	1	0.37
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	2	0.37
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	3	0.37
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	5	0.37
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	6	0.37
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	6	0.37
(2,1447)	1:57:B:SER:H	1:53:B:LEU:HB3	4	0.37
(2,1416)	1:41:B:ASP:H	1:98:B:LEU:HD11	5	0.37
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	6	0.37
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	7	0.37
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD12	8	0.37
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	4	0.37
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB3	6	0.37
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB3	7	0.37
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	1	0.37
(2,1175)	1:45:B:MET:HE3	1:40:B:PHE:HD1	2	0.37
(2,1175)	1:73:B:ILE:HG13	1:81:B:TRP:HD1	5	0.37
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB3	5	0.37
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG21	10	0.37
(2,1098)	1:98:B:LEU:HD21	1:39:B:ARG:HA	2	0.37
(2,1086)	1:59:B:LYS:H	1:59:B:LYS:HG3	4	0.37
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	6	0.37
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	5	0.37
(2,1081)	1:55:B:PRO:HD2	1:54:B:ILE:HA	2	0.37
(2,1078)	1:65:B:LEU:HD13	1:88:B:CYS:H	3	0.37
(2,984)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	9	0.37
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	7	0.37
(2,950)	1:67:B:ALA:HB1	1:66:B:TYR:HB3	3	0.37
(2,905)	1:28:B:LYS:HG3	1:31:B:ILE:HD12	6	0.37
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	1	0.37
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,888)	1:15:B:LEU:H	1:69:B:MET:HE1	9	0.37
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	10	0.37
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	2	0.37
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	5	0.37
(2,877)	1:87:B:GLU:H	1:86:B:GLY:HA2	8	0.37
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG21	4	0.37
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE2	9	0.37
(2,762)	1:13:B:ALA:HB1	1:14:B:TRP:HB2	3	0.37
(2,762)	1:13:B:ALA:HB2	1:14:B:TRP:HB2	9	0.37
(2,761)	1:13:B:ALA:HB3	1:9:B:MET:HA	2	0.37
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	1	0.37
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	7	0.37
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	7	0.37
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	9	0.37
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE2	1	0.37
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	6	0.37
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	8	0.37
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD2	4	0.37
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	10	0.37
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	1	0.37
(2,441)	1:19:B:THR:H	1:20:B:PRO:HG2	6	0.37
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD21	9	0.37
(2,364)	1:23:B:PRO:HG3	1:51:B:VAL:HG12	8	0.37
(2,232)	1:28:B:LYS:HE3	1:28:B:LYS:HB2	8	0.37
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD22	2	0.37
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD23	5	0.37
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	2	0.37
(2,158)	1:25:B:LEU:H	1:26:B:ILE:HB	10	0.37
(2,153)	1:56:B:GLU:HG3	1:53:B:LEU:HA	7	0.37
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	2	0.37
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	1	0.37
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	5	0.37
(2,104)	1:30:B:PHE:HB3	1:40:B:PHE:HE2	4	0.37
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	9	0.37
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	8	0.37
(1,866)	1:101:B:LYS:H	1:101:B:LYS:HG3	2	0.37
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB2	1	0.37
(1,812)	1:80:B:THR:HG21	1:81:B:TRP:HZ2	8	0.37
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	8	0.37
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	10	0.37
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	2	0.37
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	3	0.37
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	3	0.37
(1,392)	1:99:B:ILE:H	1:99:B:ILE:HG12	5	0.37
(1,387)	1:70:B:PRO:HG3	1:73:B:ILE:HD11	3	0.37
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	8	0.37
(1,270)	1:11:B:LYS:HB2	1:11:B:LYS:HD3	4	0.37
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	1	0.37
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD11	1	0.37
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD13	5	0.37
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD12	10	0.37
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	2	0.37
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	2	0.36
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	5	0.36
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	1	0.36
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD23	10	0.36
(2,1577)	1:19:B:THR:H	1:58:B:THR:HG21	7	0.36
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	7	0.36
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	5	0.36
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	6	0.36
(2,1392)	1:88:B:CYS:H	1:89:B:ILE:HG12	4	0.36
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	3	0.36
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	5	0.36
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG22	8	0.36
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	3	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD11	3	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD13	4	0.36
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD12	10	0.36
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	6	0.36
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	5	0.36
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD13	8	0.36
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB2	4	0.36
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	1	0.36
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	3	0.36
(2,1066)	1:101:B:LYS:H	1:99:B:ILE:HG13	9	0.36
(2,975)	1:54:B:ILE:HB	1:52:B:THR:HA	9	0.36
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	1	0.36
(2,973)	1:76:B:GLU:HG2	1:80:B:THR:HB	2	0.36
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	9	0.36
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	2	0.36
(2,886)	1:87:B:GLU:HB3	1:86:B:GLY:HA3	4	0.36
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG22	1	0.36
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,737)	1:51:B:VAL:H	1:49:B:GLN:HA	3	0.36
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	10	0.36
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	9	0.36
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	3	0.36
(2,666)	1:22:B:LEU:HD13	1:86:B:GLY:HA2	1	0.36
(2,666)	1:22:B:LEU:HD13	1:22:B:LEU:HA	7	0.36
(2,666)	1:22:B:LEU:HD13	1:22:B:LEU:HA	10	0.36
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD12	6	0.36
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD21	3	0.36
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	8	0.36
(2,596)	1:61:B:CYS:H	1:60:B:LYS:HG3	2	0.36
(2,572)	1:26:B:ILE:HA	1:30:B:PHE:HD2	9	0.36
(2,537)	1:36:B:LEU:HD23	1:35:B:ASP:HB2	2	0.36
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	10	0.36
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	1	0.36
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	2	0.36
(2,178)	1:62:B:GLN:HG3	1:19:B:THR:HG21	3	0.36
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD1	8	0.36
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	5	0.36
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	10	0.36
(2,104)	1:30:B:PHE:HB3	1:40:B:PHE:HE1	9	0.36
(2,57)	1:85:B:LEU:HB2	1:84:B:SER:HB2	7	0.36
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	6	0.36
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	6	0.36
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB1	10	0.36
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	9	0.36
(1,866)	1:101:B:LYS:H	1:101:B:LYS:HG3	10	0.36
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD11	2	0.36
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB3	3	0.36
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB1	4	0.36
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE1	8	0.36
(1,736)	1:11:B:LYS:HD2	1:66:B:TYR:HE1	9	0.36
(1,598)	1:26:B:ILE:HG22	1:90:B:GLY:HA3	3	0.36
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	6	0.36
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	4	0.36
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	5	0.36
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	8	0.36
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	9	0.36
(1,317)	1:31:B:ILE:H	1:31:B:ILE:HG12	3	0.36
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	10	0.36
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	4	0.36
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD13	2	0.36
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD11	6	0.36
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD13	7	0.36
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	1	0.36
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	7	0.36
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	8	0.36
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	10	0.36
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	1	0.36
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	1	0.35
(2,1579)	1:24:B:ASP:H	1:54:B:ILE:HD12	8	0.35
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	8	0.35
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	1	0.35
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	10	0.35
(2,1456)	1:93:B:PHE:H	1:54:B:ILE:HG23	8	0.35
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB3	1	0.35
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	9	0.35
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	5	0.35
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	4	0.35
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	1	0.35
(2,1381)	1:30:B:PHE:H	1:26:B:ILE:HB	10	0.35
(2,1362)	1:92:B:ASP:H	1:91:B:LYS:HB3	6	0.35
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE2	10	0.35
(2,1157)	1:73:B:ILE:HG21	1:14:B:TRP:HZ3	10	0.35
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB3	1	0.35
(2,1145)	1:12:B:ASP:H	1:13:B:ALA:HB1	7	0.35
(2,1066)	1:101:B:LYS:H	1:99:B:ILE:HG13	10	0.35
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG22	6	0.35
(2,1017)	1:64:B:GLU:HG3	1:60:B:LYS:HD3	2	0.35
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	9	0.35
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	9	0.35
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	3	0.35
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	1	0.35
(2,912)	1:96:B:LYS:HB2	1:96:B:LYS:HE3	3	0.35
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	3	0.35
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	10	0.35
(2,845)	1:100:B:PRO:HD3	1:101:B:LYS:HG3	4	0.35
(2,778)	1:31:B:ILE:HG21	1:32:B:GLN:HG3	3	0.35
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	2	0.35
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.35
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	1	0.35
(2,680)	1:28:B:LYS:HG2	1:28:B:LYS:HA	8	0.35
(2,666)	1:22:B:LEU:HD11	1:86:B:GLY:HA2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	10	0.35
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD1	10	0.35
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	10	0.35
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	4	0.35
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	10	0.35
(2,330)	1:39:B:ARG:HB3	1:98:B:LEU:HD21	9	0.35
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	6	0.35
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	2	0.35
(2,170)	1:62:B:GLN:HG2	1:85:B:LEU:HD21	5	0.35
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	4	0.35
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	10	0.35
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	6	0.35
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	5	0.35
(2,104)	1:30:B:PHE:HB3	1:93:B:PHE:HE2	8	0.35
(1,1306)	1:52:B:THR:H	1:53:B:LEU:HD23	4	0.35
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD12	2	0.35
(1,1062)	1:11:B:LYS:H	1:72:B:LYS:HG3	2	0.35
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD11	6	0.35
(1,1012)	1:50:B:CYS:H	1:27:B:CYS:HB3	4	0.35
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	2	0.35
(1,844)	1:54:B:ILE:HD13	1:89:B:ILE:HG23	5	0.35
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB2	2	0.35
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB1	9	0.35
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	3	0.35
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	4	0.35
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	5	0.35
(1,464)	1:98:B:LEU:HD11	1:40:B:PHE:HD2	10	0.35
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	9	0.35
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	1	0.35
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	3	0.35
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	6	0.35
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	7	0.35
(1,329)	1:44:B:LYS:HB2	1:44:B:LYS:HA	10	0.35
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD11	4	0.35
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD12	8	0.35
(1,169)	1:54:B:ILE:HB	1:54:B:ILE:HD12	9	0.35
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	9	0.35
(1,52)	1:11:B:LYS:HE2	1:69:B:MET:HB3	2	0.35
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	8	0.34
(2,1583)	1:46:B:THR:H	1:47:B:TYR:HB2	7	0.34
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG23	3	0.34
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1538)	1:72:B:LYS:H	1:70:B:PRO:HG3	2	0.34
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG23	8	0.34
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG22	8	0.34
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD22	1	0.34
(2,1310)	1:9:B:MET:H	1:9:B:MET:HB2	10	0.34
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	7	0.34
(2,1179)	1:31:B:ILE:HG13	1:27:B:CYS:HA	4	0.34
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD11	9	0.34
(2,1142)	1:9:B:MET:HG3	1:78:B:ALA:HB1	4	0.34
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG22	2	0.34
(2,1128)	1:99:B:ILE:HA	1:99:B:ILE:HG13	4	0.34
(2,1103)	1:24:B:ASP:HB2	1:21:B:LEU:HD23	2	0.34
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	9	0.34
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	1	0.34
(2,1078)	1:65:B:LEU:HD12	1:88:B:CYS:H	6	0.34
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG22	1	0.34
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD12	5	0.34
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	6	0.34
(2,877)	1:89:B:ILE:H	1:86:B:GLY:HA2	6	0.34
(2,858)	1:58:B:THR:HG23	1:23:B:PRO:HD2	4	0.34
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE1	6	0.34
(2,768)	1:64:B:GLU:HB3	1:65:B:LEU:HA	6	0.34
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	6	0.34
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG22	4	0.34
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	6	0.34
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	7	0.34
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HE2	1	0.34
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	5	0.34
(2,666)	1:22:B:LEU:HD13	1:86:B:GLY:HA2	3	0.34
(2,666)	1:22:B:LEU:HD12	1:22:B:LEU:HA	8	0.34
(2,596)	1:61:B:CYS:H	1:60:B:LYS:HG3	3	0.34
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	1	0.34
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	9	0.34
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	3	0.34
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	7	0.34
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	7	0.34
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	8	0.34
(2,391)	1:48:B:GLU:HB3	1:47:B:TYR:HD1	4	0.34
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	5	0.34
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	3	0.34
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD23	3	0.34
(2,181)	1:96:B:LYS:HE2	1:96:B:LYS:HB3	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:96:B:LYS:HE2	1:96:B:LYS:HB3	10	0.34
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	5	0.34
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	1	0.34
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	3	0.34
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB2	8	0.34
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	10	0.34
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	2	0.34
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD13	3	0.34
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	10	0.34
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	3	0.34
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB1	6	0.34
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	8	0.34
(1,728)	1:26:B:ILE:HD13	1:86:B:GLY:HA3	5	0.34
(1,728)	1:26:B:ILE:HD13	1:86:B:GLY:HA3	7	0.34
(1,728)	1:26:B:ILE:HD13	1:86:B:GLY:HA3	10	0.34
(1,703)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	4	0.34
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	5	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	1	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	2	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	3	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	4	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	5	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	6	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	7	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	8	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	9	0.34
(1,497)	1:48:B:GLU:HB2	1:48:B:GLU:HA	10	0.34
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	9	0.34
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	7	0.34
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	7	0.34
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG21	4	0.34
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	3	0.34
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	6	0.34
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HD1	8	0.33
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD13	10	0.33
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	4	0.33
(2,1600)	1:68:B:SER:H	1:65:B:LEU:HD22	7	0.33
(2,1540)	1:72:B:LYS:H	1:72:B:LYS:HG2	2	0.33
(2,1539)	1:72:B:LYS:H	1:72:B:LYS:HB3	4	0.33
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	1	0.33
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	7	0.33
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD12	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB1	9	0.33
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	9	0.33
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	7	0.33
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	6	0.33
(2,1415)	1:41:B:ASP:H	1:45:B:MET:HB2	2	0.33
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	7	0.33
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD13	2	0.33
(2,1383)	1:30:B:PHE:H	1:31:B:ILE:HD12	4	0.33
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	6	0.33
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	6	0.33
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	3	0.33
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG21	9	0.33
(2,1117)	1:-6:B:VAL:HG11	1:-4:B:ASP:H	3	0.33
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	8	0.33
(2,1095)	1:15:B:LEU:HD13	1:66:B:TYR:H	2	0.33
(2,1058)	1:44:B:LYS:HD3	1:41:B:ASP:HB3	7	0.33
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	2	0.33
(2,1029)	1:53:B:LEU:HA	1:54:B:ILE:HG12	9	0.33
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	8	0.33
(2,874)	1:26:B:ILE:HD11	1:90:B:GLY:HA3	1	0.33
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	9	0.33
(2,858)	1:58:B:THR:HG22	1:23:B:PRO:HD2	9	0.33
(2,845)	1:100:B:PRO:HD3	1:101:B:LYS:HG3	8	0.33
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG22	3	0.33
(2,776)	1:31:B:ILE:HG21	1:40:B:PHE:HE1	4	0.33
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	3	0.33
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	2	0.33
(2,713)	1:51:B:VAL:HG22	1:52:B:THR:HB	6	0.33
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD1	8	0.33
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	9	0.33
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	3	0.33
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG22	9	0.33
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	6	0.33
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	2	0.33
(2,496)	1:70:B:PRO:HG3	1:81:B:TRP:HD1	6	0.33
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE3	9	0.33
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	3	0.33
(2,453)	1:62:B:GLN:HB3	1:63:B:ASP:HB3	3	0.33
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	8	0.33
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	8	0.33
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	3	0.33
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	5	0.33
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	6	0.33
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	7	0.33
(2,181)	1:96:B:LYS:HE2	1:96:B:LYS:HB3	2	0.33
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	7	0.33
(2,158)	1:25:B:LEU:H	1:26:B:ILE:HB	8	0.33
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	8	0.33
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	9	0.33
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	6	0.33
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	1	0.33
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	4	0.33
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	8	0.33
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD3	10	0.33
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	3	0.33
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD12	7	0.33
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	4	0.33
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD13	2	0.33
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	8	0.33
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	6	0.33
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE2	1	0.33
(1,690)	1:26:B:ILE:HD12	1:30:B:PHE:HE2	5	0.33
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	8	0.33
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	7	0.33
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	1	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	1	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	2	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	3	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	4	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	5	0.33
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	8	0.33
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	9	0.33
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	5	0.33
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	5	0.33
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	6	0.33
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	10	0.32
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG22	8	0.32
(2,1436)	1:60:B:LYS:H	1:63:B:ASP:HB3	7	0.32
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	2	0.32
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	2	0.32
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	1	0.32
(2,1381)	1:30:B:PHE:H	1:28:B:LYS:HG3	2	0.32
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD11	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	10	0.32
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	8	0.32
(2,1163)	1:54:B:ILE:HD12	1:23:B:PRO:HG3	10	0.32
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG23	7	0.32
(2,1095)	1:15:B:LEU:HD12	1:66:B:TYR:H	1	0.32
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	3	0.32
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	8	0.32
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	8	0.32
(2,998)	1:74:B:ASN:HB3	1:8:B:GLU:HB2	4	0.32
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG3	8	0.32
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	9	0.32
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	10	0.32
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	6	0.32
(2,929)	1:-1:B:LYS:HE3	1:-1:B:LYS:HA	5	0.32
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD11	7	0.32
(2,889)	1:73:B:ILE:HD12	1:78:B:ALA:H	3	0.32
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	5	0.32
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	4	0.32
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG22	6	0.32
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	8	0.32
(2,737)	1:51:B:VAL:H	1:49:B:GLN:HA	1	0.32
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG21	9	0.32
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	1	0.32
(2,653)	1:39:B:ARG:HB3	1:98:B:LEU:HD13	7	0.32
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE3	8	0.32
(2,561)	1:85:B:LEU:HD13	1:14:B:TRP:HZ2	8	0.32
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	7	0.32
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	1	0.32
(2,465)	1:15:B:LEU:HG	1:12:B:ASP:HA	8	0.32
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	7	0.32
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	10	0.32
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD23	10	0.32
(2,216)	1:8:B:GLU:HB2	1:74:B:ASN:HB2	8	0.32
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	1	0.32
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	4	0.32
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	8	0.32
(2,189)	1:60:B:LYS:HB3	1:60:B:LYS:HG3	10	0.32
(2,169)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	7	0.32
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD2	10	0.32
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG23	2	0.32
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	9	0.32
(2,91)	1:90:B:GLY:H	1:93:B:PHE:HB3	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:71:B:ASP:HB2	1:72:B:LYS:HG3	9	0.32
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	2	0.32
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	9	0.32
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	2	0.32
(2,42)	1:28:B:LYS:H	1:28:B:LYS:HE3	1	0.32
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	2	0.32
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	8	0.32
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	7	0.32
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	8	0.32
(1,1218)	1:98:B:LEU:H	1:94:B:ALA:HB1	4	0.32
(1,1137)	1:60:B:LYS:H	1:60:B:LYS:HE3	2	0.32
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG12	10	0.32
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	6	0.32
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD11	1	0.32
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	3	0.32
(1,841)	1:54:B:ILE:HD12	1:23:B:PRO:HB3	9	0.32
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	4	0.32
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	4	0.32
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	1	0.32
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	9	0.32
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	10	0.32
(1,529)	1:59:B:LYS:HD2	1:59:B:LYS:HA	10	0.32
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	2	0.32
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	9	0.32
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	2	0.32
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	6	0.32
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	5	0.32
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	8	0.32
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	2	0.32
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	3	0.32
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	5	0.32
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	3	0.32
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	8	0.32
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	2	0.32
(1,155)	1:95:B:GLU:H	1:95:B:GLU:HG2	4	0.32
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	1	0.32
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	8	0.32
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	4	0.31
(2,1591)	1:17:B:SER:H	1:15:B:LEU:HD23	3	0.31
(2,1540)	1:72:B:LYS:H	1:72:B:LYS:HG2	6	0.31
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	2	0.31
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	9	0.31
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD13	6	0.31
(2,1439)	1:22:B:LEU:H	1:18:B:MET:HG3	9	0.31
(2,1434)	1:22:B:LEU:H	1:58:B:THR:HB	8	0.31
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	3	0.31
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	7	0.31
(2,1347)	1:99:B:ILE:H	1:99:B:ILE:HD13	2	0.31
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	4	0.31
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	2	0.31
(2,1275)	1:62:B:GLN:H	1:59:B:LYS:HD3	4	0.31
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD13	9	0.31
(2,1240)	1:87:B:GLU:H	1:83:B:ARG:HB2	6	0.31
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB1	1	0.31
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB2	6	0.31
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB2	9	0.31
(2,1163)	1:54:B:ILE:HD13	1:23:B:PRO:HG3	7	0.31
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG23	1	0.31
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG23	1	0.31
(2,1098)	1:98:B:LEU:HD21	1:39:B:ARG:HA	9	0.31
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	1	0.31
(2,1030)	1:44:B:LYS:HD3	1:41:B:ASP:HB2	5	0.31
(2,1028)	1:38:B:LYS:HD2	1:39:B:ARG:H	2	0.31
(2,992)	1:8:B:GLU:HB3	1:73:B:ILE:H	9	0.31
(2,985)	1:62:B:GLN:HG3	1:59:B:LYS:HD3	6	0.31
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	5	0.31
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB3	6	0.31
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	9	0.31
(2,890)	1:11:B:LYS:H	1:73:B:ILE:HD12	6	0.31
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	3	0.31
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	8	0.31
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	1	0.31
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	10	0.31
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	8	0.31
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG22	8	0.31
(2,762)	1:9:B:MET:HE1	1:14:B:TRP:HB2	6	0.31
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	5	0.31
(2,713)	1:51:B:VAL:HG21	1:52:B:THR:HB	8	0.31
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	10	0.31
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	5	0.31
(2,565)	1:15:B:LEU:HD21	1:62:B:GLN:HA	10	0.31
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	9	0.31
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	2	0.31
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	4	0.31
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	5	0.31
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	7	0.31
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	8	0.31
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	10	0.31
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	4	0.31
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	5	0.31
(2,268)	1:45:B:MET:HG2	1:53:B:LEU:HD11	7	0.31
(2,187)	1:97:B:HIS:HB3	1:43:B:ILE:HG13	3	0.31
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	10	0.31
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	1	0.31
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	6	0.31
(2,144)	1:87:B:GLU:HG3	1:91:B:LYS:HD3	2	0.31
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	7	0.31
(2,103)	1:30:B:PHE:HB3	1:40:B:PHE:HD1	3	0.31
(2,81)	1:71:B:ASP:HB2	1:72:B:LYS:HG3	1	0.31
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	6	0.31
(2,38)	1:-1:B:LYS:HE3	1:-1:B:LYS:HB2	3	0.31
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	9	0.31
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	7	0.31
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	5	0.31
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD11	6	0.31
(1,827)	1:89:B:ILE:HG23	1:93:B:PHE:HD2	7	0.31
(1,771)	1:43:B:ILE:H	1:45:B:MET:HB3	2	0.31
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	9	0.31
(1,697)	1:85:B:LEU:H	1:82:B:GLY:HA3	6	0.31
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG21	5	0.31
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	10	0.31
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	2	0.31
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	10	0.31
(1,362)	1:34:B:PRO:HB2	1:34:B:PRO:HA	9	0.31
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	6	0.31
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE1	6	0.31
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE1	8	0.31
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	6	0.31
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	2	0.31
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	3	0.31
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	9	0.31
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	10	0.31
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HD1	7	0.3
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD13	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	9	0.3
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	4	0.3
(2,1484)	1:95:B:GLU:H	1:99:B:ILE:HG23	5	0.3
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD11	1	0.3
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD11	9	0.3
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB2	10	0.3
(2,1440)	1:60:B:LYS:H	1:63:B:ASP:HB2	10	0.3
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	3	0.3
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG23	3	0.3
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	8	0.3
(2,1369)	1:58:B:THR:H	1:59:B:LYS:HD3	9	0.3
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	5	0.3
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	3	0.3
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	10	0.3
(2,1163)	1:54:B:ILE:HD13	1:23:B:PRO:HG3	5	0.3
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG22	2	0.3
(2,1158)	1:31:B:ILE:HD13	1:27:B:CYS:HB3	4	0.3
(2,1157)	1:73:B:ILE:HG21	1:14:B:TRP:HZ3	6	0.3
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD13	1	0.3
(2,1153)	1:27:B:CYS:H	1:54:B:ILE:HG23	3	0.3
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG23	1	0.3
(2,1142)	1:9:B:MET:HG3	1:78:B:ALA:HB2	7	0.3
(2,1141)	1:17:B:SER:H	1:13:B:ALA:HB2	1	0.3
(2,1140)	1:57:B:SER:H	1:89:B:ILE:HG23	9	0.3
(2,1111)	1:19:B:THR:HG21	1:15:B:LEU:HB3	8	0.3
(2,1078)	1:65:B:LEU:HD12	1:88:B:CYS:H	4	0.3
(2,1066)	1:101:B:LYS:H	1:99:B:ILE:HG13	8	0.3
(2,1054)	1:54:B:ILE:HA	1:26:B:ILE:HG13	1	0.3
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	5	0.3
(2,1043)	1:33:B:ASP:H	1:37:B:LYS:HD3	10	0.3
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	6	0.3
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	3	0.3
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	1	0.3
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	5	0.3
(2,933)	1:24:B:ASP:HB3	1:23:B:PRO:HB2	6	0.3
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	3	0.3
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	4	0.3
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	8	0.3
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	2	0.3
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	5	0.3
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	6	0.3
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	2	0.3
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	4	0.3
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	7	0.3
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	8	0.3
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	4	0.3
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG23	5	0.3
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD1	6	0.3
(2,776)	1:31:B:ILE:HG23	1:40:B:PHE:HE2	3	0.3
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	6	0.3
(2,688)	1:38:B:LYS:HA	1:38:B:LYS:HE2	9	0.3
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	5	0.3
(2,680)	1:28:B:LYS:HG2	1:28:B:LYS:HA	7	0.3
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD1	9	0.3
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD22	8	0.3
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE3	5	0.3
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	2	0.3
(2,545)	1:17:B:SER:HB2	1:14:B:TRP:HD1	5	0.3
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	1	0.3
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	4	0.3
(2,416)	1:81:B:TRP:HB2	1:80:B:THR:HB	9	0.3
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	10	0.3
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	7	0.3
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	9	0.3
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	3	0.3
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	2	0.3
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	4	0.3
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	6	0.3
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	7	0.3
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	7	0.3
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	2	0.3
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	6	0.3
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	7	0.3
(2,261)	1:45:B:MET:HG3	1:53:B:LEU:HD13	1	0.3
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD11	2	0.3
(2,131)	1:40:B:PHE:HB2	1:98:B:LEU:HD12	7	0.3
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	1	0.3
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	3	0.3
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	2	0.3
(2,81)	1:71:B:ASP:HB2	1:72:B:LYS:HG3	6	0.3
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	8	0.3
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	8	0.3
(1,1318)	1:43:B:ILE:H	1:39:B:ARG:HG2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG11	8	0.3
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	4	0.3
(1,1006)	1:94:B:ALA:H	1:96:B:LYS:HB3	1	0.3
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	9	0.3
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	5	0.3
(1,615)	1:43:B:ILE:HD11	1:98:B:LEU:HA	6	0.3
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD11	1	0.3
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	9	0.3
(1,485)	1:98:B:LEU:HD23	1:40:B:PHE:HB3	6	0.3
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	6	0.3
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG21	6	0.3
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG23	7	0.3
(1,282)	1:60:B:LYS:HD3	1:57:B:SER:HA	5	0.3
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	7	0.3
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	8	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	2	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	3	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	5	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	6	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	9	0.3
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	10	0.3
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	9	0.3
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	4	0.3
(1,82)	1:74:B:ASN:H	1:74:B:ASN:HB2	3	0.3
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	4	0.3
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	5	0.3
(1,38)	1:98:B:LEU:H	1:98:B:LEU:HB3	7	0.3
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	3	0.29
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	6	0.29
(2,1605)	1:97:B:HIS:H	1:98:B:LEU:HD23	4	0.29
(2,1517)	1:61:B:CYS:H	1:60:B:LYS:HG3	3	0.29
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	1	0.29
(2,1489)	1:27:B:CYS:H	1:27:B:CYS:HB3	3	0.29
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	9	0.29
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	9	0.29
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD11	6	0.29
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD12	7	0.29
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG21	3	0.29
(2,1275)	1:62:B:GLN:H	1:60:B:LYS:HG3	1	0.29
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE2	8	0.29
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	9	0.29
(2,1088)	1:-1:B:LYS:HG2	1:-2:B:ASP:HA	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1080)	1:73:B:ILE:HG13	1:78:B:ALA:HA	9	0.29
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD11	4	0.29
(2,950)	1:67:B:ALA:HB3	1:66:B:TYR:HB3	5	0.29
(2,912)	1:96:B:LYS:HB2	1:96:B:LYS:HE3	6	0.29
(2,905)	1:28:B:LYS:HG3	1:31:B:ILE:HD12	5	0.29
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	1	0.29
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	7	0.29
(2,862)	1:70:B:PRO:HB2	1:70:B:PRO:HD3	10	0.29
(2,858)	1:58:B:THR:HG23	1:23:B:PRO:HD2	5	0.29
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	5	0.29
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	9	0.29
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG22	7	0.29
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	1	0.29
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG21	6	0.29
(2,746)	1:39:B:ARG:HG2	1:39:B:ARG:HA	4	0.29
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG21	1	0.29
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	3	0.29
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	8	0.29
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE2	6	0.29
(2,608)	1:85:B:LEU:HD21	1:62:B:GLN:HB2	10	0.29
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	1	0.29
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	5	0.29
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	3	0.29
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	3	0.29
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	4	0.29
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	6	0.29
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	4	0.29
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	4	0.29
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	8	0.29
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	7	0.29
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	9	0.29
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	4	0.29
(1,1169)	1:51:B:VAL:H	1:27:B:CYS:HB3	4	0.29
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG11	2	0.29
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD11	5	0.29
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	1	0.29
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB3	5	0.29
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	6	0.29
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	5	0.29
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD13	2	0.29
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE2	4	0.29
(1,660)	1:74:B:ASN:HB3	1:74:B:ASN:HA	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD13	3	0.29
(1,603)	1:30:B:PHE:H	1:26:B:ILE:HG23	3	0.29
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG21	5	0.29
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	3	0.29
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	8	0.29
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	4	0.29
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	5	0.29
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	6	0.29
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	2	0.29
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	1	0.29
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	7	0.29
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	8	0.29
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	8	0.29
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	9	0.29
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	4	0.29
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	7	0.29
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	1	0.29
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	1	0.29
(1,52)	1:11:B:LYS:HE2	1:69:B:MET:HB3	1	0.29
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	3	0.28
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	2	0.28
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	3	0.28
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	6	0.28
(2,1489)	1:35:B:ASP:H	1:35:B:ASP:HB3	5	0.28
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD13	5	0.28
(2,1451)	1:93:B:PHE:H	1:26:B:ILE:HG13	6	0.28
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	2	0.28
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	7	0.28
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	10	0.28
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	6	0.28
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	7	0.28
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB2	4	0.28
(2,1163)	1:54:B:ILE:HD11	1:23:B:PRO:HG3	1	0.28
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG21	6	0.28
(2,1099)	1:21:B:LEU:H	1:21:B:LEU:HD22	10	0.28
(2,1072)	1:28:B:LYS:HG3	1:27:B:CYS:HB3	8	0.28
(2,1054)	1:54:B:ILE:HA	1:26:B:ILE:HG13	6	0.28
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG3	1	0.28
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG2	3	0.28
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	2	0.28
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	1	0.28
(2,946)	1:41:B:ASP:HB3	1:42:B:GLU:HG2	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	5	0.28
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE1	4	0.28
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	2	0.28
(2,768)	1:64:B:GLU:HB3	1:65:B:LEU:HA	8	0.28
(2,715)	1:51:B:VAL:HG11	1:27:B:CYS:HB3	4	0.28
(2,680)	1:28:B:LYS:HG2	1:28:B:LYS:HA	10	0.28
(2,565)	1:15:B:LEU:HD22	1:62:B:GLN:HA	8	0.28
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	7	0.28
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	5	0.28
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	4	0.28
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	6	0.28
(2,514)	1:22:B:LEU:HD23	1:82:B:GLY:HA3	7	0.28
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	2	0.28
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	9	0.28
(2,453)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	4	0.28
(2,453)	1:6:B:PRO:HG2	1:5:B:ASN:HB2	9	0.28
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	8	0.28
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	4	0.28
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD3	4	0.28
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	4	0.28
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	9	0.28
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	10	0.28
(2,281)	1:18:B:MET:HG2	1:18:B:MET:HA	1	0.28
(2,216)	1:8:B:GLU:HB2	1:74:B:ASN:HB2	4	0.28
(2,163)	1:63:B:ASP:H	1:62:B:GLN:HG2	5	0.28
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	6	0.28
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	9	0.28
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	3	0.28
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	2	0.28
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	9	0.28
(2,39)	1:33:B:ASP:HB2	1:36:B:LEU:HD22	1	0.28
(2,22)	1:61:B:CYS:HB3	1:61:B:CYS:HA	1	0.28
(2,18)	1:98:B:LEU:HB3	1:39:B:ARG:HD3	9	0.28
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	10	0.28
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	1	0.28
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG22	3	0.28
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD12	1	0.28
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	10	0.28
(1,1072)	1:64:B:GLU:H	1:63:B:ASP:HB3	5	0.28
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD21	1	0.28
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD23	10	0.28
(1,895)	1:33:B:ASP:H	1:33:B:ASP:HB3	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD11	7	0.28
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB3	7	0.28
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	9	0.28
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	4	0.28
(1,811)	1:18:B:MET:H	1:19:B:THR:HG23	5	0.28
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	9	0.28
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD13	4	0.28
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	7	0.28
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	10	0.28
(1,568)	1:89:B:ILE:HG22	1:57:B:SER:HB2	2	0.28
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	1	0.28
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	8	0.28
(1,377)	1:58:B:THR:H	1:57:B:SER:HB2	10	0.28
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG23	3	0.28
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG22	10	0.28
(1,278)	1:64:B:GLU:HB3	1:61:B:CYS:HB3	5	0.28
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	5	0.28
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	7	0.28
(1,206)	1:45:B:MET:HB3	1:45:B:MET:HG3	4	0.28
(1,203)	1:97:B:HIS:HB2	1:93:B:PHE:HD1	1	0.28
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE3	10	0.28
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	1	0.28
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	6	0.28
(1,160)	1:95:B:GLU:HG3	1:95:B:GLU:HA	10	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	2	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	3	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	4	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	5	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	6	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	7	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	8	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	9	0.28
(1,151)	1:48:B:GLU:HG2	1:48:B:GLU:HB2	10	0.28
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	9	0.27
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	7	0.27
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	5	0.27
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD11	3	0.27
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD11	10	0.27
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB2	8	0.27
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	10	0.27
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD12	9	0.27
(2,1320)	1:40:B:PHE:H	1:38:B:LYS:HB3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1313)	1:50:B:CYS:H	1:40:B:PHE:HE1	3	0.27
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG22	3	0.27
(2,1229)	1:83:B:ARG:H	1:78:B:ALA:HB3	7	0.27
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	2	0.27
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	10	0.27
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG22	2	0.27
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	1	0.27
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	5	0.27
(2,1072)	1:28:B:LYS:HG3	1:32:B:GLN:HG3	7	0.27
(2,1072)	1:28:B:LYS:HG3	1:32:B:GLN:HG3	10	0.27
(2,1005)	1:9:B:MET:HG2	1:8:B:GLU:HG3	9	0.27
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	2	0.27
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	4	0.27
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	6	0.27
(2,954)	1:16:B:ASN:HB3	1:15:B:LEU:HB2	1	0.27
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	5	0.27
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	8	0.27
(2,892)	1:77:B:THR:HB	1:73:B:ILE:HD12	1	0.27
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	9	0.27
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB2	9	0.27
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB3	10	0.27
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	3	0.27
(2,841)	1:20:B:PRO:HD3	1:20:B:PRO:HA	6	0.27
(2,822)	1:73:B:ILE:HG23	1:75:B:SER:HA	8	0.27
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG23	3	0.27
(2,768)	1:64:B:GLU:HB3	1:65:B:LEU:HA	9	0.27
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	7	0.27
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	9	0.27
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE2	7	0.27
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD2	2	0.27
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE2	8	0.27
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	10	0.27
(2,548)	1:11:B:LYS:HE3	1:66:B:TYR:HA	10	0.27
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	8	0.27
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	7	0.27
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	5	0.27
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	6	0.27
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	6	0.27
(2,365)	1:33:B:ASP:H	1:32:B:GLN:HB3	10	0.27
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	1	0.27
(2,332)	1:55:B:PRO:HG3	1:51:B:VAL:HA	2	0.27
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,320)	1:39:B:ARG:HD2	1:39:B:ARG:HB2	9	0.27
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	3	0.27
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD22	10	0.27
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	9	0.27
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	8	0.27
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	10	0.27
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	4	0.27
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	10	0.27
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	4	0.27
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD11	4	0.27
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG23	5	0.27
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG22	7	0.27
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	2	0.27
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	10	0.27
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD13	4	0.27
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD13	9	0.27
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD13	3	0.27
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	8	0.27
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	4	0.27
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	9	0.27
(1,1006)	1:94:B:ALA:H	1:96:B:LYS:HB3	10	0.27
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD12	1	0.27
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	6	0.27
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB2	8	0.27
(1,811)	1:18:B:MET:H	1:19:B:THR:HG22	2	0.27
(1,766)	1:99:B:ILE:HG21	1:101:B:LYS:HB3	3	0.27
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG22	8	0.27
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	5	0.27
(1,656)	1:31:B:ILE:HD11	1:40:B:PHE:HE1	10	0.27
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD13	2	0.27
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD11	5	0.27
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	8	0.27
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	5	0.27
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	6	0.27
(1,312)	1:54:B:ILE:HG12	1:54:B:ILE:HG23	1	0.27
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	3	0.27
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	5	0.27
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	10	0.27
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD13	3	0.26
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG21	6	0.26
(2,1540)	1:96:B:LYS:H	1:96:B:LYS:HG2	1	0.26
(2,1540)	1:72:B:LYS:H	1:72:B:LYS:HG2	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	2	0.26
(2,1492)	1:25:B:LEU:H	1:25:B:LEU:HB3	10	0.26
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD11	3	0.26
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD12	2	0.26
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB1	3	0.26
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB1	5	0.26
(2,1451)	1:93:B:PHE:H	1:98:B:LEU:HG	1	0.26
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	3	0.26
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	3	0.26
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD11	2	0.26
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE2	4	0.26
(2,1234)	1:73:B:ILE:H	1:72:B:LYS:HE2	5	0.26
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	1	0.26
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	10	0.26
(2,1159)	1:97:B:HIS:HB2	1:43:B:ILE:HG23	3	0.26
(2,1149)	1:91:B:LYS:H	1:89:B:ILE:HG23	2	0.26
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	1	0.26
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	2	0.26
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	4	0.26
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	5	0.26
(2,1112)	1:37:B:LYS:HB3	1:37:B:LYS:HA	7	0.26
(2,1095)	1:12:B:ASP:H	1:15:B:LEU:HD13	5	0.26
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD12	10	0.26
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	2	0.26
(2,1048)	1:96:B:LYS:HD3	1:53:B:LEU:HA	8	0.26
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD11	6	0.26
(2,953)	1:66:B:TYR:HB3	1:62:B:GLN:HG2	2	0.26
(2,937)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	8	0.26
(2,934)	1:24:B:ASP:HB3	1:21:B:LEU:HB3	3	0.26
(2,934)	1:24:B:ASP:HB3	1:21:B:LEU:HB3	4	0.26
(2,889)	1:73:B:ILE:HD11	1:78:B:ALA:H	6	0.26
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB2	1	0.26
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB1	7	0.26
(2,848)	1:39:B:ARG:HD2	1:100:B:PRO:HD2	1	0.26
(2,737)	1:51:B:VAL:H	1:49:B:GLN:HA	5	0.26
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	3	0.26
(2,720)	1:85:B:LEU:HG	1:85:B:LEU:HA	4	0.26
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD2	4	0.26
(2,666)	1:22:B:LEU:HD13	1:86:B:GLY:HA2	4	0.26
(2,608)	1:85:B:LEU:HD23	1:62:B:GLN:HB2	2	0.26
(2,583)	1:21:B:LEU:HD13	1:17:B:SER:HB3	10	0.26
(2,565)	1:15:B:LEU:HD21	1:62:B:GLN:HA	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	2	0.26
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	5	0.26
(2,480)	1:87:B:GLU:H	1:83:B:ARG:HG3	10	0.26
(2,462)	1:34:B:PRO:HG2	1:35:B:ASP:H	8	0.26
(2,454)	1:62:B:GLN:HB3	1:63:B:ASP:HB2	6	0.26
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	5	0.26
(2,266)	1:45:B:MET:HG3	1:40:B:PHE:HE2	7	0.26
(2,249)	1:23:B:PRO:HB2	1:54:B:ILE:HG22	9	0.26
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	5	0.26
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	8	0.26
(2,174)	1:52:B:THR:H	1:49:B:GLN:HG3	6	0.26
(2,144)	1:56:B:GLU:HG3	1:53:B:LEU:HG	4	0.26
(2,128)	1:40:B:PHE:HB2	1:36:B:LEU:HA	7	0.26
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	3	0.26
(2,39)	1:61:B:CYS:HB2	1:89:B:ILE:HD12	6	0.26
(2,17)	1:92:B:ASP:HB3	1:57:B:SER:HA	6	0.26
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD21	2	0.26
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	8	0.26
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	4	0.26
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	1	0.26
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	7	0.26
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD21	7	0.26
(1,844)	1:54:B:ILE:HD12	1:89:B:ILE:HG21	9	0.26
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD12	1	0.26
(1,811)	1:18:B:MET:H	1:19:B:THR:HG21	3	0.26
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	1	0.26
(1,759)	1:35:B:ASP:HB2	1:36:B:LEU:HG	4	0.26
(1,656)	1:31:B:ILE:HD11	1:40:B:PHE:HE2	8	0.26
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	8	0.26
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG23	1	0.26
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG21	3	0.26
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG22	4	0.26
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD11	2	0.26
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	3	0.26
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	8	0.26
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	9	0.26
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	10	0.26
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	7	0.26
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	7	0.26
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HD1	1	0.25
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG21	4	0.25
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD13	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1458)	1:93:B:PHE:H	1:26:B:ILE:HG22	5	0.25
(2,1439)	1:60:B:LYS:H	1:59:B:LYS:HG3	2	0.25
(2,1434)	1:60:B:LYS:H	1:57:B:SER:HB3	1	0.25
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD12	3	0.25
(2,1392)	1:88:B:CYS:H	1:89:B:ILE:HG12	8	0.25
(2,1381)	1:30:B:PHE:H	1:28:B:LYS:HG3	9	0.25
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	9	0.25
(2,1290)	1:91:B:LYS:H	1:87:B:GLU:HG2	2	0.25
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD12	7	0.25
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	2	0.25
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	4	0.25
(2,1165)	1:54:B:ILE:HD12	1:50:B:CYS:HB2	4	0.25
(2,1163)	1:54:B:ILE:HD11	1:23:B:PRO:HG3	6	0.25
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB2	5	0.25
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	2	0.25
(2,1030)	1:44:B:LYS:HD3	1:41:B:ASP:HB2	7	0.25
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG2	10	0.25
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	9	0.25
(2,969)	1:76:B:GLU:HG2	1:80:B:THR:H	8	0.25
(2,963)	1:101:B:LYS:H	1:99:B:ILE:HB	6	0.25
(2,909)	1:99:B:ILE:HD11	1:95:B:GLU:HG2	7	0.25
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD13	8	0.25
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	3	0.25
(2,897)	1:69:B:MET:HE3	1:11:B:LYS:HE2	5	0.25
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD1	1	0.25
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	9	0.25
(2,769)	1:65:B:LEU:HB2	1:65:B:LEU:HA	10	0.25
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	8	0.25
(2,696)	1:28:B:LYS:HG2	1:28:B:LYS:HA	8	0.25
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE2	2	0.25
(2,643)	1:96:B:LYS:HB3	1:93:B:PHE:HA	4	0.25
(2,640)	1:40:B:PHE:HA	1:98:B:LEU:HA	7	0.25
(2,634)	1:98:B:LEU:HD11	1:30:B:PHE:HE1	8	0.25
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE3	10	0.25
(2,608)	1:85:B:LEU:HD23	1:62:B:GLN:HB2	8	0.25
(2,572)	1:33:B:ASP:H	1:31:B:ILE:HA	4	0.25
(2,556)	1:45:B:MET:HE3	1:98:B:LEU:HA	2	0.25
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	1	0.25
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	9	0.25
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HZ	4	0.25
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD23	8	0.25
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	7	0.25
(2,330)	1:39:B:ARG:HB3	1:98:B:LEU:HD21	2	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	1	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	2	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	3	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	6	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	7	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	8	0.25
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	9	0.25
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	1	0.25
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD12	2	0.25
(2,286)	1:65:B:LEU:HB2	1:64:B:GLU:HB3	3	0.25
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD22	4	0.25
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	2	0.25
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD22	3	0.25
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	2	0.25
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	6	0.25
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	8	0.25
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	10	0.25
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	3	0.25
(1,1137)	1:60:B:LYS:H	1:60:B:LYS:HE3	6	0.25
(1,1137)	1:60:B:LYS:H	1:60:B:LYS:HE3	10	0.25
(1,1080)	1:28:B:LYS:H	1:51:B:VAL:HG12	6	0.25
(1,942)	1:87:B:GLU:H	1:65:B:LEU:HD12	9	0.25
(1,895)	1:33:B:ASP:H	1:33:B:ASP:HB3	1	0.25
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG22	6	0.25
(1,568)	1:89:B:ILE:HG23	1:57:B:SER:HB2	9	0.25
(1,455)	1:85:B:LEU:HD22	1:85:B:LEU:H	8	0.25
(1,382)	1:39:B:ARG:HG2	1:39:B:ARG:HA	4	0.25
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	1	0.25
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	2	0.25
(1,324)	1:81:B:TRP:H	1:81:B:TRP:HB3	7	0.25
(1,272)	1:64:B:GLU:H	1:64:B:GLU:HB3	3	0.25
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	2	0.25
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	4	0.25
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	1	0.24
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HD1	2	0.24
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	4	0.24
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	1	0.24
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD12	4	0.24
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	8	0.24
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD21	10	0.24
(2,1456)	1:93:B:PHE:H	1:54:B:ILE:HG23	9	0.24
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	8	0.24
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	9	0.24
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	9	0.24
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	4	0.24
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	8	0.24
(2,1269)	1:54:B:ILE:H	1:53:B:LEU:HD13	9	0.24
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	8	0.24
(2,1183)	1:14:B:TRP:HE1	1:9:B:MET:HB2	7	0.24
(2,1179)	1:31:B:ILE:HG13	1:27:B:CYS:HA	3	0.24
(2,1163)	1:54:B:ILE:HD13	1:23:B:PRO:HG3	3	0.24
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG21	4	0.24
(2,1148)	1:20:B:PRO:HD3	1:16:B:ASN:HA	8	0.24
(2,1124)	1:51:B:VAL:HG11	1:23:B:PRO:HG2	5	0.24
(2,1112)	1:37:B:LYS:HD3	1:37:B:LYS:HA	9	0.24
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	1	0.24
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	4	0.24
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD12	5	0.24
(2,1082)	1:73:B:ILE:HG13	1:78:B:ALA:HA	9	0.24
(2,1066)	1:101:B:LYS:H	1:99:B:ILE:HG13	4	0.24
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD12	10	0.24
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	5	0.24
(2,1018)	1:22:B:LEU:H	1:18:B:MET:HG3	1	0.24
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG2	2	0.24
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	5	0.24
(2,973)	1:87:B:GLU:HG3	1:84:B:SER:HB3	6	0.24
(2,969)	1:96:B:LYS:H	1:95:B:GLU:HG3	3	0.24
(2,969)	1:76:B:GLU:HG2	1:80:B:THR:H	7	0.24
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	8	0.24
(2,925)	1:83:B:ARG:H	1:83:B:ARG:HD2	3	0.24
(2,901)	1:74:B:ASN:H	1:73:B:ILE:HD11	10	0.24
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	3	0.24
(2,769)	1:53:B:LEU:HB2	1:53:B:LEU:HA	1	0.24
(2,713)	1:51:B:VAL:HG12	1:24:B:ASP:HA	2	0.24
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	3	0.24
(2,642)	1:43:B:ILE:HB	1:40:B:PHE:HA	1	0.24
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD23	7	0.24
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB2	2	0.24
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	3	0.24
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	3	0.24
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD2	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	8	0.24
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	9	0.24
(2,323)	1:32:B:GLN:HB3	1:32:B:GLN:H	4	0.24
(2,232)	1:28:B:LYS:HE3	1:28:B:LYS:HB2	7	0.24
(2,216)	1:8:B:GLU:HB2	1:7:B:ASN:HB3	9	0.24
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	7	0.24
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD1	3	0.24
(2,164)	1:62:B:GLN:HG3	1:66:B:TYR:HD1	7	0.24
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	3	0.24
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	6	0.24
(2,124)	1:39:B:ARG:H	1:40:B:PHE:HB3	8	0.24
(2,96)	1:93:B:PHE:HB2	1:96:B:LYS:HB2	3	0.24
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	8	0.24
(2,41)	1:61:B:CYS:HB2	1:89:B:ILE:HD13	7	0.24
(1,1320)	1:43:B:ILE:H	1:43:B:ILE:HG21	9	0.24
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB1	5	0.24
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	6	0.24
(1,1072)	1:64:B:GLU:H	1:63:B:ASP:HB3	4	0.24
(1,1068)	1:30:B:PHE:H	1:31:B:ILE:HG12	1	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	2	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD21	3	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD22	6	0.24
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD22	10	0.24
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD13	4	0.24
(1,895)	1:33:B:ASP:H	1:33:B:ASP:HB3	4	0.24
(1,615)	1:43:B:ILE:HD11	1:98:B:LEU:HA	7	0.24
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG22	7	0.24
(1,500)	1:36:B:LEU:HD13	1:36:B:LEU:HA	6	0.24
(1,500)	1:36:B:LEU:HD11	1:36:B:LEU:HA	7	0.24
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	4	0.24
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	6	0.24
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	3	0.23
(2,1628)	1:29:B:GLY:H	1:27:B:CYS:HB2	4	0.23
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	9	0.23
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	6	0.23
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD11	6	0.23
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	5	0.23
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	6	0.23
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD21	7	0.23
(2,1458)	1:93:B:PHE:H	1:26:B:ILE:HG22	8	0.23
(2,1439)	1:60:B:LYS:H	1:59:B:LYS:HG3	1	0.23
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	4	0.23
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD21	6	0.23
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	9	0.23
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	3	0.23
(2,1112)	1:37:B:LYS:HD3	1:37:B:LYS:HA	8	0.23
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD13	9	0.23
(2,1095)	1:15:B:LEU:HD13	1:66:B:TYR:H	7	0.23
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	3	0.23
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	8	0.23
(2,1078)	1:65:B:LEU:HD12	1:88:B:CYS:H	7	0.23
(2,1039)	1:49:B:GLN:HB2	1:46:B:THR:HG21	6	0.23
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD13	3	0.23
(2,1033)	1:26:B:ILE:HG12	1:23:B:PRO:HA	10	0.23
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	7	0.23
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	10	0.23
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	8	0.23
(2,919)	1:96:B:LYS:HG3	1:96:B:LYS:HA	5	0.23
(2,907)	1:100:B:PRO:HD2	1:99:B:ILE:HD12	4	0.23
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	2	0.23
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	5	0.23
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	2	0.23
(2,814)	1:94:B:ALA:HA	1:93:B:PHE:HE1	3	0.23
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	2	0.23
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	1	0.23
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD1	6	0.23
(2,636)	1:43:B:ILE:HB	1:98:B:LEU:HD23	2	0.23
(2,608)	1:85:B:LEU:HD22	1:62:B:GLN:HB2	4	0.23
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB1	10	0.23
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE1	5	0.23
(2,566)	1:43:B:ILE:HB	1:45:B:MET:HE3	2	0.23
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	7	0.23
(2,561)	1:85:B:LEU:HD13	1:14:B:TRP:HZ2	9	0.23
(2,494)	1:83:B:ARG:HG3	1:87:B:GLU:HG2	6	0.23
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	2	0.23
(2,479)	1:39:B:ARG:HG3	1:100:B:PRO:HD3	8	0.23
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	5	0.23
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	9	0.23
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	10	0.23
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	8	0.23
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	10	0.23
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	2	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	2	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	3	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	4	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	5	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	6	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	7	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	8	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	9	0.23
(2,356)	1:32:B:GLN:HB2	1:32:B:GLN:HA	10	0.23
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	5	0.23
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	4	0.23
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	2	0.23
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	5	0.23
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	9	0.23
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	3	0.23
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	7	0.23
(2,41)	1:37:B:LYS:HE3	1:31:B:ILE:HG23	2	0.23
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD3	3	0.23
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD3	8	0.23
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD13	5	0.23
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	1	0.23
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	7	0.23
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	9	0.23
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	7	0.23
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	5	0.23
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD11	3	0.23
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB1	5	0.23
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB2	10	0.23
(1,811)	1:18:B:MET:H	1:19:B:THR:HG23	7	0.23
(1,797)	1:81:B:TRP:HB2	1:85:B:LEU:HD21	6	0.23
(1,738)	1:54:B:ILE:H	1:53:B:LEU:HB3	9	0.23
(1,650)	1:43:B:ILE:HG22	1:97:B:HIS:HB3	9	0.23
(1,615)	1:43:B:ILE:HD12	1:98:B:LEU:HA	2	0.23
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG21	2	0.23
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	5	0.23
(1,464)	1:98:B:LEU:HD13	1:40:B:PHE:HD1	3	0.23
(1,448)	1:72:B:LYS:H	1:72:B:LYS:HG2	5	0.23
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	6	0.23
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD12	6	0.23
(1,203)	1:97:B:HIS:HB2	1:93:B:PHE:HD2	5	0.23
(1,175)	1:62:B:GLN:HG3	1:62:B:GLN:HA	5	0.23
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	1	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	2	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	3	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	4	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	5	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	7	0.23
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	9	0.23
(1,102)	1:5:B:ASN:HB2	1:6:B:PRO:HD2	5	0.23
(2,1620)	1:82:B:GLY:H	1:83:B:ARG:HG3	6	0.22
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	7	0.22
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	9	0.22
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	2	0.22
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	5	0.22
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	7	0.22
(2,1454)	1:93:B:PHE:H	1:94:B:ALA:HB2	4	0.22
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	10	0.22
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	1	0.22
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	9	0.22
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	2	0.22
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG23	1	0.22
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG21	6	0.22
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	3	0.22
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	10	0.22
(2,1361)	1:92:B:ASP:H	1:60:B:LYS:HE3	3	0.22
(2,1324)	1:40:B:PHE:H	1:98:B:LEU:HD11	3	0.22
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	5	0.22
(2,1157)	1:73:B:ILE:HG22	1:14:B:TRP:HH2	7	0.22
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG22	10	0.22
(2,1112)	1:37:B:LYS:HD3	1:37:B:LYS:HA	3	0.22
(2,1057)	1:20:B:PRO:HG2	1:18:B:MET:H	1	0.22
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD11	1	0.22
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD13	7	0.22
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	4	0.22
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	10	0.22
(2,889)	1:73:B:ILE:HD11	1:78:B:ALA:H	8	0.22
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	7	0.22
(2,845)	1:100:B:PRO:HD3	1:101:B:LYS:HG3	9	0.22
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	8	0.22
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	9	0.22
(2,820)	1:9:B:MET:H	1:73:B:ILE:HG23	8	0.22
(2,785)	1:54:B:ILE:HG21	1:23:B:PRO:HD3	8	0.22
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG22	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,715)	1:51:B:VAL:HG13	1:27:B:CYS:HB3	5	0.22
(2,713)	1:51:B:VAL:HG12	1:24:B:ASP:HA	7	0.22
(2,606)	1:85:B:LEU:HD23	1:66:B:TYR:H	4	0.22
(2,593)	1:73:B:ILE:HG12	1:73:B:ILE:HA	7	0.22
(2,573)	1:37:B:LYS:HE2	1:31:B:ILE:HA	7	0.22
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	7	0.22
(2,454)	1:62:B:GLN:HB3	1:63:B:ASP:HB2	4	0.22
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	2	0.22
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	3	0.22
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	8	0.22
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	6	0.22
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	6	0.22
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	1	0.22
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	2	0.22
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD2	3	0.22
(2,316)	1:22:B:LEU:HB3	1:23:B:PRO:HA	5	0.22
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD13	8	0.22
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	8	0.22
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	1	0.22
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	2	0.22
(2,216)	1:8:B:GLU:HB2	1:74:B:ASN:HB2	3	0.22
(2,188)	1:0:B:MET:HB3	1:-1:B:LYS:H	3	0.22
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD2	2	0.22
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	10	0.22
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	3	0.22
(2,65)	1:72:B:LYS:HE3	1:72:B:LYS:HG3	7	0.22
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	4	0.22
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	5	0.22
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	10	0.22
(2,8)	1:84:B:SER:H	1:83:B:ARG:HD2	2	0.22
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD21	1	0.22
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD23	8	0.22
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	9	0.22
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	5	0.22
(1,1220)	1:98:B:LEU:H	1:99:B:ILE:HG12	2	0.22
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB2	9	0.22
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	8	0.22
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD13	7	0.22
(1,1052)	1:58:B:THR:H	1:54:B:ILE:HD12	10	0.22
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB3	8	0.22
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG21	7	0.22
(1,824)	1:99:B:ILE:HG22	1:101:B:LYS:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	4	0.22
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE1	3	0.22
(1,703)	1:85:B:LEU:HD11	1:82:B:GLY:HA3	3	0.22
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	1	0.22
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE2	10	0.22
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	6	0.22
(1,213)	1:35:B:ASP:H	1:34:B:PRO:HB3	10	0.22
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	4	0.22
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	6	0.22
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	8	0.22
(1,147)	1:48:B:GLU:HG3	1:48:B:GLU:HB3	10	0.22
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	5	0.22
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	8	0.22
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	10	0.22
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG23	1	0.21
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD11	7	0.21
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	3	0.21
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	1	0.21
(2,1493)	1:25:B:LEU:H	1:26:B:ILE:HG13	9	0.21
(2,1478)	1:27:B:CYS:H	1:54:B:ILE:HG22	8	0.21
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	9	0.21
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	3	0.21
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	1	0.21
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	10	0.21
(2,1137)	1:24:B:ASP:HA	1:28:B:LYS:HG3	8	0.21
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	6	0.21
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD11	1	0.21
(2,1039)	1:49:B:GLN:HB2	1:46:B:THR:HG23	1	0.21
(2,1028)	1:38:B:LYS:HD3	1:39:B:ARG:H	9	0.21
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	6	0.21
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE3	10	0.21
(2,929)	1:-1:B:LYS:HE2	1:-1:B:LYS:HA	1	0.21
(2,910)	1:31:B:ILE:HD12	1:47:B:TYR:HD1	9	0.21
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE3	4	0.21
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE3	5	0.21
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE2	8	0.21
(2,874)	1:26:B:ILE:HD11	1:90:B:GLY:HA3	4	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	3	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	4	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	5	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	6	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	8	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	9	0.21
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	10	0.21
(2,778)	1:31:B:ILE:HG23	1:32:B:GLN:HG3	10	0.21
(2,756)	1:-1:B:LYS:HD3	1:-1:B:LYS:HA	8	0.21
(2,735)	1:92:B:ASP:HA	1:95:B:GLU:HB2	9	0.21
(2,720)	1:22:B:LEU:HG	1:22:B:LEU:HA	2	0.21
(2,719)	1:56:B:GLU:HA	1:56:B:GLU:HG2	10	0.21
(2,696)	1:28:B:LYS:HG2	1:28:B:LYS:HA	7	0.21
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	2	0.21
(2,668)	1:58:B:THR:HA	1:22:B:LEU:HD12	9	0.21
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG21	2	0.21
(2,583)	1:21:B:LEU:HD11	1:17:B:SER:HB3	5	0.21
(2,561)	1:85:B:LEU:HD11	1:14:B:TRP:HZ2	5	0.21
(2,556)	1:45:B:MET:HE1	1:98:B:LEU:HA	3	0.21
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	9	0.21
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	5	0.21
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	1	0.21
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	6	0.21
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	7	0.21
(2,430)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	5	0.21
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	9	0.21
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	5	0.21
(2,359)	1:54:B:ILE:H	1:23:B:PRO:HG3	9	0.21
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD2	9	0.21
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD12	1	0.21
(2,169)	1:62:B:GLN:HG2	1:59:B:LYS:HD2	3	0.21
(2,164)	1:62:B:GLN:HG2	1:66:B:TYR:HD2	1	0.21
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	5	0.21
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	3	0.21
(2,103)	1:30:B:PHE:HB3	1:40:B:PHE:HD2	5	0.21
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	7	0.21
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	4	0.21
(2,38)	1:60:B:LYS:HE2	1:60:B:LYS:HB2	1	0.21
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	6	0.21
(2,17)	1:92:B:ASP:HB3	1:57:B:SER:HA	9	0.21
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB3	2	0.21
(1,1318)	1:43:B:ILE:H	1:39:B:ARG:HG2	10	0.21
(1,1252)	1:19:B:THR:H	1:18:B:MET:HG3	8	0.21
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	3	0.21
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	6	0.21
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD11	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	6	0.21
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG23	6	0.21
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB1	9	0.21
(1,828)	1:17:B:SER:H	1:13:B:ALA:HB2	1	0.21
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	7	0.21
(1,762)	1:89:B:ILE:HG13	1:88:B:CYS:HB3	1	0.21
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB2	1	0.21
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	3	0.21
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB3	5	0.21
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB3	10	0.21
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	8	0.21
(1,728)	1:26:B:ILE:HD12	1:86:B:GLY:HA3	9	0.21
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD11	4	0.21
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG23	10	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	1	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	2	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	4	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	5	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	8	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	9	0.21
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	10	0.21
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	8	0.21
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE2	4	0.21
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	5	0.21
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	10	0.21
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD22	1	0.21
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	1	0.21
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	6	0.2
(2,1644)	1:83:B:ARG:H	1:80:B:THR:HG22	4	0.2
(2,1643)	1:89:B:ILE:H	1:89:B:ILE:HD12	1	0.2
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG22	2	0.2
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG22	10	0.2
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	1	0.2
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD12	5	0.2
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	1	0.2
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	6	0.2
(2,1477)	1:65:B:LEU:H	1:15:B:LEU:HD21	4	0.2
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	10	0.2
(2,1418)	1:41:B:ASP:H	1:39:B:ARG:HB3	10	0.2
(2,1385)	1:64:B:GLU:H	1:60:B:LYS:HG3	5	0.2
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	9	0.2
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1243)	1:87:B:GLU:H	1:89:B:ILE:HD11	6	0.2
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	1	0.2
(2,1138)	1:38:B:LYS:HG2	1:36:B:LEU:HA	9	0.2
(2,1133)	1:36:B:LEU:HG	1:30:B:PHE:HA	8	0.2
(2,1097)	1:98:B:LEU:HD22	1:39:B:ARG:HA	1	0.2
(2,1095)	1:15:B:LEU:HD12	1:66:B:TYR:H	8	0.2
(2,1064)	1:36:B:LEU:HG	1:30:B:PHE:HD2	2	0.2
(2,1039)	1:49:B:GLN:HB2	1:46:B:THR:HG23	10	0.2
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG21	9	0.2
(2,967)	1:56:B:GLU:HG2	1:96:B:LYS:HE3	9	0.2
(2,935)	1:83:B:ARG:HA	1:85:B:LEU:HB2	2	0.2
(2,926)	1:61:B:CYS:HB3	1:64:B:GLU:HB2	1	0.2
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	2	0.2
(2,874)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	2	0.2
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	1	0.2
(2,812)	1:65:B:LEU:HB2	1:65:B:LEU:HA	2	0.2
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	2	0.2
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG23	1	0.2
(2,724)	1:81:B:TRP:HA	1:80:B:THR:HG23	2	0.2
(2,720)	1:22:B:LEU:HG	1:22:B:LEU:HA	9	0.2
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	8	0.2
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD2	3	0.2
(2,676)	1:28:B:LYS:HA	1:47:B:TYR:HD2	5	0.2
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	4	0.2
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	5	0.2
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	6	0.2
(2,632)	1:23:B:PRO:HG2	1:58:B:THR:HG23	1	0.2
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE3	9	0.2
(2,606)	1:85:B:LEU:HD23	1:66:B:TYR:H	7	0.2
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	4	0.2
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	6	0.2
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	8	0.2
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	10	0.2
(2,537)	1:36:B:LEU:HD21	1:35:B:ASP:HB2	9	0.2
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	10	0.2
(2,525)	1:98:B:LEU:H	1:45:B:MET:HE3	10	0.2
(2,496)	1:53:B:LEU:HG	1:93:B:PHE:HD1	1	0.2
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	4	0.2
(2,435)	1:51:B:VAL:HA	1:52:B:THR:HA	10	0.2
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	3	0.2
(2,374)	1:23:B:PRO:HG2	1:20:B:PRO:HB2	7	0.2
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,332)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	3	0.2
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	1	0.2
(2,257)	1:54:B:ILE:H	1:23:B:PRO:HB3	7	0.2
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	9	0.2
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	10	0.2
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	2	0.2
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	9	0.2
(2,87)	1:74:B:ASN:HB3	1:8:B:GLU:HB3	6	0.2
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	6	0.2
(2,62)	1:21:B:LEU:HB2	1:20:B:PRO:HD2	3	0.2
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	7	0.2
(2,17)	1:92:B:ASP:HB3	1:57:B:SER:HA	5	0.2
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	4	0.2
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD11	5	0.2
(1,1006)	1:94:B:ALA:H	1:96:B:LYS:HB3	5	0.2
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB3	1	0.2
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB1	10	0.2
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG21	1	0.2
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG23	4	0.2
(1,844)	1:54:B:ILE:HD13	1:89:B:ILE:HG23	3	0.2
(1,824)	1:99:B:ILE:HG21	1:101:B:LYS:HA	2	0.2
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	7	0.2
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	7	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	2	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	6	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	7	0.2
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB2	8	0.2
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	10	0.2
(1,656)	1:31:B:ILE:HD13	1:40:B:PHE:HE1	6	0.2
(1,605)	1:42:B:GLU:HB2	1:43:B:ILE:HD12	6	0.2
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG22	9	0.2
(1,558)	1:101:B:LYS:HB2	1:101:B:LYS:HA	6	0.2
(1,485)	1:98:B:LEU:HD22	1:40:B:PHE:HB3	7	0.2
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD22	5	0.2
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	6	0.2
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	6	0.2
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	3	0.2
(1,373)	1:92:B:ASP:HB2	1:57:B:SER:HB3	7	0.2
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	6	0.2
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	9	0.2
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE1	4	0.2
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:-6:B:VAL:HB	1:-6:B:VAL:HA	3	0.2
(1,166)	1:54:B:ILE:HB	1:55:B:PRO:HD2	2	0.2
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	4	0.2
(1,52)	1:11:B:LYS:HE2	1:69:B:MET:HB3	7	0.2
(2,1601)	1:97:B:HIS:H	1:99:B:ILE:HA	8	0.19
(2,1538)	1:96:B:LYS:H	1:99:B:ILE:HB	4	0.19
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD13	6	0.19
(2,1478)	1:27:B:CYS:H	1:54:B:ILE:HG22	10	0.19
(2,1474)	1:63:B:ASP:H	1:59:B:LYS:HD3	4	0.19
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	10	0.19
(2,1420)	1:41:B:ASP:H	1:37:B:LYS:HB2	4	0.19
(2,1419)	1:41:B:ASP:H	1:38:B:LYS:HB2	5	0.19
(2,1415)	1:41:B:ASP:H	1:43:B:ILE:HG13	8	0.19
(2,1392)	1:88:B:CYS:H	1:26:B:ILE:HD12	10	0.19
(2,1214)	1:36:B:LEU:H	1:38:B:LYS:HB2	8	0.19
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	8	0.19
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	9	0.19
(2,1179)	1:31:B:ILE:HG13	1:27:B:CYS:HA	9	0.19
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG22	8	0.19
(2,1137)	1:24:B:ASP:HA	1:28:B:LYS:HG3	10	0.19
(2,1119)	1:36:B:LEU:HG	1:30:B:PHE:HA	8	0.19
(2,1096)	1:40:B:PHE:HB2	1:98:B:LEU:HD11	6	0.19
(2,1087)	1:60:B:LYS:H	1:59:B:LYS:HG2	9	0.19
(2,1085)	1:37:B:LYS:H	1:37:B:LYS:HG3	7	0.19
(2,1045)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	3	0.19
(2,1044)	1:95:B:GLU:HB2	1:99:B:ILE:HD11	3	0.19
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	3	0.19
(2,966)	1:95:B:GLU:HG2	1:99:B:ILE:HG12	2	0.19
(2,952)	1:50:B:CYS:HB3	1:49:B:GLN:HB3	5	0.19
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	6	0.19
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	9	0.19
(2,897)	1:69:B:MET:HE3	1:11:B:LYS:HE2	10	0.19
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	1	0.19
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	8	0.19
(2,801)	1:89:B:ILE:HD11	1:86:B:GLY:HA3	6	0.19
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG23	1	0.19
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG21	6	0.19
(2,771)	1:18:B:MET:HG2	1:18:B:MET:HA	9	0.19
(2,731)	1:15:B:LEU:HB2	1:15:B:LEU:HA	8	0.19
(2,696)	1:28:B:LYS:HG2	1:28:B:LYS:HA	10	0.19
(2,694)	1:28:B:LYS:HA	1:32:B:GLN:HG3	3	0.19
(2,687)	1:38:B:LYS:HA	1:41:B:ASP:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,687)	1:38:B:LYS:HA	1:41:B:ASP:H	10	0.19
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	1	0.19
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	7	0.19
(2,640)	1:-6:B:VAL:HA	1:-5:B:ASP:HA	1	0.19
(2,565)	1:15:B:LEU:HD23	1:62:B:GLN:HA	1	0.19
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	1	0.19
(2,546)	1:84:B:SER:HB3	1:84:B:SER:HA	7	0.19
(2,527)	1:73:B:ILE:HG12	1:73:B:ILE:HA	8	0.19
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	10	0.19
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	6	0.19
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	9	0.19
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	5	0.19
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	6	0.19
(2,220)	1:18:B:MET:HB3	1:15:B:LEU:HD22	7	0.19
(2,175)	1:46:B:THR:H	1:49:B:GLN:HG2	5	0.19
(2,168)	1:54:B:ILE:HB	1:51:B:VAL:HG12	8	0.19
(2,154)	1:95:B:GLU:HG3	1:99:B:ILE:HG13	8	0.19
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	3	0.19
(2,112)	1:73:B:ILE:HB	1:8:B:GLU:HG3	4	0.19
(2,76)	1:-5:B:ASP:H	1:-5:B:ASP:HB3	7	0.19
(2,62)	1:21:B:LEU:HB2	1:20:B:PRO:HD2	10	0.19
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	4	0.19
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	7	0.19
(2,35)	1:89:B:ILE:H	1:61:B:CYS:HB2	10	0.19
(2,6)	1:69:B:MET:H	1:65:B:LEU:HB3	3	0.19
(2,3)	1:65:B:LEU:HB2	1:62:B:GLN:HA	5	0.19
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD12	10	0.19
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB1	10	0.19
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	2	0.19
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	2	0.19
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB2	2	0.19
(1,960)	1:69:B:MET:H	1:67:B:ALA:HB2	7	0.19
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG22	5	0.19
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB3	1	0.19
(1,831)	1:4:B:ALA:HB3	1:5:B:ASN:HA	1	0.19
(1,820)	1:81:B:TRP:H	1:80:B:THR:HG23	6	0.19
(1,809)	1:52:B:THR:HG21	1:52:B:THR:HB	2	0.19
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	3	0.19
(1,809)	1:52:B:THR:HG23	1:52:B:THR:HB	4	0.19
(1,809)	1:52:B:THR:HG21	1:52:B:THR:HB	5	0.19
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	8	0.19
(1,809)	1:52:B:THR:HG23	1:52:B:THR:HB	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB1	4	0.19
(1,744)	1:67:B:ALA:HA	1:67:B:ALA:HB2	9	0.19
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	1	0.19
(1,631)	1:43:B:ILE:HD11	1:100:B:PRO:HD3	9	0.19
(1,591)	1:32:B:GLN:H	1:31:B:ILE:HG21	8	0.19
(1,590)	1:78:B:ALA:HB2	1:73:B:ILE:HG22	5	0.19
(1,426)	1:33:B:ASP:HB2	1:36:B:LEU:HD21	4	0.19
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	6	0.19
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	10	0.19
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	3	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	1	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	2	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	3	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	5	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	8	0.19
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	10	0.19
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE3	8	0.19
(2,1656)	1:84:B:SER:H	1:81:B:TRP:HZ3	10	0.18
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD12	6	0.18
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD11	9	0.18
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	2	0.18
(2,1439)	1:60:B:LYS:H	1:59:B:LYS:HG3	3	0.18
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	5	0.18
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	8	0.18
(2,1420)	1:41:B:ASP:H	1:39:B:ARG:HG3	5	0.18
(2,1339)	1:-2:B:ASP:H	1:-3:B:ASP:HB3	7	0.18
(2,1337)	1:94:B:ALA:H	1:26:B:ILE:HG22	5	0.18
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	4	0.18
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	7	0.18
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	10	0.18
(2,1163)	1:54:B:ILE:HD13	1:23:B:PRO:HG3	2	0.18
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD13	8	0.18
(2,1044)	1:95:B:GLU:HB2	1:99:B:ILE:HD11	5	0.18
(2,1039)	1:49:B:GLN:HB3	1:46:B:THR:HG23	5	0.18
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	5	0.18
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	4	0.18
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	8	0.18
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	3	0.18
(2,828)	1:44:B:LYS:H	1:43:B:ILE:HG21	10	0.18
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG23	1	0.18
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG22	8	0.18
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,737)	1:51:B:VAL:H	1:49:B:GLN:HA	9	0.18
(2,720)	1:22:B:LEU:HG	1:22:B:LEU:HA	1	0.18
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	4	0.18
(2,713)	1:51:B:VAL:HG11	1:24:B:ASP:HA	5	0.18
(2,712)	1:51:B:VAL:HG13	1:47:B:TYR:HE1	2	0.18
(2,712)	1:51:B:VAL:HG13	1:47:B:TYR:HE1	4	0.18
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	10	0.18
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	6	0.18
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	8	0.18
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	10	0.18
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB1	5	0.18
(2,596)	1:91:B:LYS:HG3	1:92:B:ASP:H	8	0.18
(2,554)	1:89:B:ILE:H	1:85:B:LEU:HD13	6	0.18
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	5	0.18
(2,501)	1:98:B:LEU:HG	1:30:B:PHE:HD1	6	0.18
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	4	0.18
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	3	0.18
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	8	0.18
(2,471)	1:39:B:ARG:HG3	1:39:B:ARG:HA	6	0.18
(2,454)	1:61:B:CYS:HB3	1:65:B:LEU:HG	7	0.18
(2,430)	1:101:B:LYS:HD2	1:99:B:ILE:HG21	7	0.18
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	1	0.18
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	4	0.18
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	5	0.18
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	7	0.18
(2,423)	1:44:B:LYS:H	1:44:B:LYS:HB3	8	0.18
(2,409)	1:56:B:GLU:HG2	1:96:B:LYS:HD2	8	0.18
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	8	0.18
(2,299)	1:64:B:GLU:HB2	1:65:B:LEU:H	3	0.18
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD11	9	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	1	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	2	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	3	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	4	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	5	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	7	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	8	0.18
(2,244)	1:6:B:PRO:HB2	1:6:B:PRO:HA	9	0.18
(2,244)	1:20:B:PRO:HB2	1:20:B:PRO:HA	10	0.18
(2,178)	1:49:B:GLN:HG3	1:52:B:THR:HG22	10	0.18
(2,138)	1:95:B:GLU:HG2	1:99:B:ILE:HG13	3	0.18
(2,120)	1:16:B:ASN:HB3	1:17:B:SER:HB2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:12:B:ASP:HB2	1:10:B:THR:HB	7	0.18
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	5	0.18
(2,27)	1:24:B:ASP:HB3	1:25:B:LEU:HD13	9	0.18
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD22	5	0.18
(1,1307)	1:31:B:ILE:H	1:30:B:PHE:HB3	3	0.18
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	1	0.18
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	8	0.18
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD13	2	0.18
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD12	7	0.18
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD22	8	0.18
(1,1036)	1:42:B:GLU:H	1:43:B:ILE:HD12	9	0.18
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG21	2	0.18
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG22	3	0.18
(1,838)	1:27:B:CYS:H	1:54:B:ILE:HD13	9	0.18
(1,820)	1:81:B:TRP:H	1:80:B:THR:HG23	5	0.18
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	1	0.18
(1,809)	1:52:B:THR:HG23	1:52:B:THR:HB	6	0.18
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	7	0.18
(1,809)	1:52:B:THR:HG22	1:52:B:THR:HB	9	0.18
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	3	0.18
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG22	9	0.18
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	2	0.18
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	2	0.18
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	3	0.18
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	5	0.18
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	9	0.18
(1,715)	1:82:B:GLY:HA2	1:14:B:TRP:HZ2	6	0.18
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	1	0.18
(1,476)	1:98:B:LEU:HD22	1:40:B:PHE:HD1	9	0.18
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	4	0.18
(1,360)	1:20:B:PRO:HB2	1:20:B:PRO:HA	7	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	1	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	2	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	3	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	4	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	5	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	6	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	8	0.18
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	10	0.18
(1,215)	1:6:B:PRO:HB2	1:6:B:PRO:HA	9	0.18
(1,187)	1:97:B:HIS:H	1:96:B:LYS:HB3	9	0.18
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD12	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1605)	1:97:B:HIS:H	1:98:B:LEU:HD23	9	0.17
(2,1580)	1:24:B:ASP:H	1:25:B:LEU:HB2	5	0.17
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD11	10	0.17
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	7	0.17
(2,1532)	1:98:B:LEU:H	1:45:B:MET:HE1	8	0.17
(2,1490)	1:35:B:ASP:H	1:36:B:LEU:HB2	10	0.17
(2,1451)	1:93:B:PHE:H	1:98:B:LEU:HG	3	0.17
(2,1440)	1:60:B:LYS:H	1:63:B:ASP:HB2	8	0.17
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	6	0.17
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	8	0.17
(2,1434)	1:60:B:LYS:H	1:57:B:SER:HB3	5	0.17
(2,1434)	1:22:B:LEU:H	1:19:B:THR:HB	6	0.17
(2,1422)	1:41:B:ASP:H	1:45:B:MET:HB2	2	0.17
(2,1405)	1:26:B:ILE:H	1:54:B:ILE:HG22	5	0.17
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG21	7	0.17
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	5	0.17
(2,1153)	1:61:B:CYS:H	1:89:B:ILE:HD12	6	0.17
(2,1149)	1:27:B:CYS:H	1:54:B:ILE:HG22	10	0.17
(2,1148)	1:20:B:PRO:HD3	1:16:B:ASN:HA	3	0.17
(2,1142)	1:9:B:MET:HG2	1:78:B:ALA:HB3	2	0.17
(2,1112)	1:37:B:LYS:HD3	1:37:B:LYS:HA	6	0.17
(2,1110)	1:62:B:GLN:HG3	1:19:B:THR:HG21	3	0.17
(2,1094)	1:3:B:THR:HA	1:4:B:ALA:HB2	1	0.17
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD13	5	0.17
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	2	0.17
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	10	0.17
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	8	0.17
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	2	0.17
(2,919)	1:96:B:LYS:HG3	1:96:B:LYS:HA	2	0.17
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	8	0.17
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	10	0.17
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB3	4	0.17
(2,833)	1:8:B:GLU:HB2	1:74:B:ASN:HA	9	0.17
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	6	0.17
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	9	0.17
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD1	10	0.17
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	5	0.17
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	10	0.17
(2,785)	1:54:B:ILE:HG21	1:23:B:PRO:HD3	5	0.17
(2,768)	1:56:B:GLU:HG3	1:53:B:LEU:HA	2	0.17
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB1	9	0.17
(2,713)	1:51:B:VAL:HG11	1:24:B:ASP:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,713)	1:51:B:VAL:HG12	1:24:B:ASP:HA	9	0.17
(2,709)	1:51:B:VAL:HG22	1:52:B:THR:HA	10	0.17
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	4	0.17
(2,640)	1:-6:B:VAL:HA	1:-5:B:ASP:HA	5	0.17
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	10	0.17
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	2	0.17
(2,546)	1:17:B:SER:HB3	1:17:B:SER:HA	3	0.17
(2,537)	1:85:B:LEU:HD12	1:81:B:TRP:HB3	10	0.17
(2,530)	1:66:B:TYR:HA	1:66:B:TYR:HD1	3	0.17
(2,494)	1:83:B:ARG:HG3	1:87:B:GLU:HG2	8	0.17
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	5	0.17
(2,430)	1:101:B:LYS:HD2	1:99:B:ILE:HG23	4	0.17
(2,373)	1:23:B:PRO:HG2	1:24:B:ASP:H	4	0.17
(2,373)	1:101:B:LYS:H	1:101:B:LYS:HD2	8	0.17
(2,355)	1:61:B:CYS:H	1:89:B:ILE:HG13	5	0.17
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	6	0.17
(2,332)	1:55:B:PRO:HG3	1:51:B:VAL:HA	7	0.17
(2,332)	1:40:B:PHE:HB2	1:37:B:LYS:HD3	8	0.17
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	7	0.17
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	4	0.17
(2,216)	1:8:B:GLU:HB3	1:7:B:ASN:HB3	1	0.17
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG22	7	0.17
(2,104)	1:30:B:PHE:HB3	1:93:B:PHE:HE1	2	0.17
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	8	0.17
(2,91)	1:90:B:GLY:H	1:93:B:PHE:HB3	7	0.17
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	1	0.17
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	2	0.17
(2,29)	1:25:B:LEU:HB2	1:22:B:LEU:HA	9	0.17
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB3	5	0.17
(1,1318)	1:43:B:ILE:H	1:39:B:ARG:HG2	4	0.17
(1,1269)	1:10:B:THR:H	1:72:B:LYS:HG3	9	0.17
(1,1267)	1:17:B:SER:H	1:21:B:LEU:HD12	10	0.17
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	5	0.17
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB1	3	0.17
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB2	6	0.17
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	3	0.17
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	7	0.17
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	4	0.17
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD1	5	0.17
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	9	0.17
(1,1103)	1:44:B:LYS:H	1:45:B:MET:HB3	1	0.17
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:40:B:PHE:H	1:39:B:ARG:HG2	4	0.17
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD21	7	0.17
(1,942)	1:87:B:GLU:H	1:65:B:LEU:HD13	3	0.17
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG23	10	0.17
(1,834)	1:95:B:GLU:HG2	1:94:B:ALA:HB1	2	0.17
(1,831)	1:4:B:ALA:HB2	1:5:B:ASN:HA	7	0.17
(1,820)	1:81:B:TRP:H	1:80:B:THR:HG22	4	0.17
(1,814)	1:33:B:ASP:HB2	1:30:B:PHE:HA	10	0.17
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	8	0.17
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	6	0.17
(1,728)	1:26:B:ILE:HD12	1:86:B:GLY:HA3	1	0.17
(1,653)	1:31:B:ILE:HD13	1:47:B:TYR:HA	4	0.17
(1,589)	1:78:B:ALA:HB3	1:14:B:TRP:HD1	3	0.17
(1,477)	1:98:B:LEU:HD21	1:93:B:PHE:HE2	6	0.17
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD12	2	0.17
(1,400)	1:28:B:LYS:HG3	1:28:B:LYS:HA	10	0.17
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	7	0.17
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	8	0.17
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	7	0.17
(1,319)	1:31:B:ILE:HB	1:31:B:ILE:HG12	9	0.17
(1,243)	1:45:B:MET:HG3	1:45:B:MET:HE3	7	0.17
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	3	0.17
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	4	0.16
(2,1506)	1:95:B:GLU:H	1:96:B:LYS:HB2	10	0.16
(2,1453)	1:93:B:PHE:H	1:91:B:LYS:HB2	1	0.16
(2,1440)	1:22:B:LEU:H	1:24:B:ASP:HB2	3	0.16
(2,1440)	1:60:B:LYS:H	1:63:B:ASP:HB2	6	0.16
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	4	0.16
(2,1270)	1:54:B:ILE:H	1:51:B:VAL:HG13	6	0.16
(2,1253)	1:37:B:LYS:H	1:38:B:LYS:HG3	7	0.16
(2,1221)	1:85:B:LEU:H	1:85:B:LEU:HD12	6	0.16
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	7	0.16
(2,1163)	1:54:B:ILE:HD12	1:23:B:PRO:HG3	8	0.16
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	4	0.16
(2,1032)	1:23:B:PRO:HB2	1:23:B:PRO:HA	9	0.16
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	3	0.16
(2,963)	1:101:B:LYS:H	1:99:B:ILE:HB	3	0.16
(2,946)	1:41:B:ASP:HB3	1:42:B:GLU:HG2	4	0.16
(2,946)	1:41:B:ASP:HB3	1:42:B:GLU:HG2	5	0.16
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	6	0.16
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	9	0.16
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	4	0.16
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	7	0.16
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	10	0.16
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG22	5	0.16
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG22	5	0.16
(2,720)	1:22:B:LEU:HG	1:22:B:LEU:HA	5	0.16
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	1	0.16
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	8	0.16
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	4	0.16
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	2	0.16
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	3	0.16
(2,608)	1:85:B:LEU:HD23	1:62:B:GLN:HB2	3	0.16
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	1	0.16
(2,572)	1:26:B:ILE:HA	1:30:B:PHE:HD2	6	0.16
(2,571)	1:66:B:TYR:HA	1:68:B:SER:H	5	0.16
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	6	0.16
(2,528)	1:22:B:LEU:HD22	1:86:B:GLY:HA3	7	0.16
(2,528)	1:22:B:LEU:HD22	1:86:B:GLY:HA3	10	0.16
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	4	0.16
(2,471)	1:39:B:ARG:HG3	1:39:B:ARG:HA	1	0.16
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	3	0.16
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD13	5	0.16
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	2	0.16
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	7	0.16
(2,153)	1:76:B:GLU:HG2	1:77:B:THR:HA	2	0.16
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG23	5	0.16
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD11	10	0.16
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	2	0.16
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	5	0.16
(1,1150)	1:93:B:PHE:H	1:93:B:PHE:HD2	10	0.16
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD21	10	0.16
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG21	9	0.16
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB1	3	0.16
(1,824)	1:99:B:ILE:HG23	1:101:B:LYS:HA	6	0.16
(1,812)	1:80:B:THR:HG23	1:81:B:TRP:HZ2	4	0.16
(1,811)	1:18:B:MET:H	1:19:B:THR:HG22	10	0.16
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG22	6	0.16
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	1	0.16
(1,742)	1:72:B:LYS:HG2	1:71:B:ASP:HB3	7	0.16
(1,723)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	10	0.16
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB3	6	0.16
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:71:B:ASP:HA	1:11:B:LYS:HD3	5	0.16
(1,500)	1:36:B:LEU:HD12	1:36:B:LEU:HA	4	0.16
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE1	4	0.16
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE1	7	0.16
(1,477)	1:98:B:LEU:HD21	1:93:B:PHE:HE2	8	0.16
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD13	10	0.16
(1,406)	1:53:B:LEU:HG	1:53:B:LEU:HA	1	0.16
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	7	0.16
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	2	0.16
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	4	0.16
(1,238)	1:77:B:THR:HB	1:73:B:ILE:HD12	1	0.16
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	2	0.16
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	7	0.16
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD11	3	0.15
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	8	0.15
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	2	0.15
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	3	0.15
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	4	0.15
(2,1434)	1:60:B:LYS:H	1:57:B:SER:HB3	7	0.15
(2,1376)	1:30:B:PHE:H	1:31:B:ILE:HA	7	0.15
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	1	0.15
(2,1270)	1:54:B:ILE:H	1:51:B:VAL:HG12	8	0.15
(2,1241)	1:87:B:GLU:H	1:89:B:ILE:HB	4	0.15
(2,1236)	1:73:B:ILE:H	1:72:B:LYS:HB2	1	0.15
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	4	0.15
(2,1154)	1:99:B:ILE:HG22	1:101:B:LYS:HA	7	0.15
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	1	0.15
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	7	0.15
(2,1089)	1:97:B:HIS:H	1:45:B:MET:HE1	3	0.15
(2,1054)	1:26:B:ILE:HG13	1:90:B:GLY:HA2	2	0.15
(2,1031)	1:51:B:VAL:HA	1:23:B:PRO:HA	3	0.15
(2,1022)	1:89:B:ILE:HG13	1:58:B:THR:HG23	2	0.15
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	5	0.15
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	9	0.15
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	5	0.15
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	6	0.15
(2,909)	1:99:B:ILE:HD13	1:95:B:GLU:HG2	4	0.15
(2,887)	1:86:B:GLY:HA3	1:85:B:LEU:HB3	6	0.15
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB2	5	0.15
(2,831)	1:74:B:ASN:HA	1:73:B:ILE:HA	5	0.15
(2,786)	1:23:B:PRO:HB3	1:54:B:ILE:HG23	7	0.15
(2,785)	1:54:B:ILE:HG23	1:23:B:PRO:HD3	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,768)	1:64:B:GLU:HB3	1:65:B:LEU:HA	5	0.15
(2,720)	1:85:B:LEU:HG	1:85:B:LEU:HA	7	0.15
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	6	0.15
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	5	0.15
(2,717)	1:65:B:LEU:H	1:64:B:GLU:HA	6	0.15
(2,713)	1:51:B:VAL:HG12	1:24:B:ASP:HA	4	0.15
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	3	0.15
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	5	0.15
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	6	0.15
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	7	0.15
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	10	0.15
(2,688)	1:91:B:LYS:HA	1:91:B:LYS:HE3	6	0.15
(2,658)	1:27:B:CYS:HB2	1:27:B:CYS:HA	3	0.15
(2,658)	1:27:B:CYS:HB2	1:27:B:CYS:HA	5	0.15
(2,646)	1:61:B:CYS:H	1:61:B:CYS:HA	9	0.15
(2,614)	1:77:B:THR:HA	1:77:B:THR:HG23	9	0.15
(2,608)	1:85:B:LEU:HD21	1:62:B:GLN:HB2	5	0.15
(2,596)	1:61:B:CYS:H	1:60:B:LYS:HG3	5	0.15
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	9	0.15
(2,571)	1:66:B:TYR:HA	1:68:B:SER:H	6	0.15
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	9	0.15
(2,476)	1:14:B:TRP:HZ3	1:15:B:LEU:HG	8	0.15
(2,475)	1:34:B:PRO:HA	1:37:B:LYS:HG2	2	0.15
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	2	0.15
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	8	0.15
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	10	0.15
(2,428)	1:20:B:PRO:HG2	1:21:B:LEU:HD22	10	0.15
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	2	0.15
(2,377)	1:22:B:LEU:H	1:23:B:PRO:HG2	9	0.15
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	4	0.15
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD11	7	0.15
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	4	0.15
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	8	0.15
(2,249)	1:100:B:PRO:HB3	1:43:B:ILE:HG23	2	0.15
(2,219)	1:18:B:MET:HB3	1:15:B:LEU:HA	8	0.15
(2,202)	1:45:B:MET:HB2	1:40:B:PHE:HA	6	0.15
(2,175)	1:46:B:THR:H	1:49:B:GLN:HG2	8	0.15
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE3	6	0.15
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE2	8	0.15
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE2	10	0.15
(2,153)	1:76:B:GLU:HG2	1:77:B:THR:HA	6	0.15
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG21	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	5	0.15
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	6	0.15
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	9	0.15
(2,105)	1:30:B:PHE:HB3	1:98:B:LEU:HD12	1	0.15
(2,86)	1:77:B:THR:H	1:74:B:ASN:HB3	3	0.15
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	9	0.15
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	9	0.15
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	5	0.15
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD21	9	0.15
(2,5)	1:65:B:LEU:HB2	1:15:B:LEU:HD22	10	0.15
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD11	6	0.15
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB3	2	0.15
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	6	0.15
(1,1121)	1:44:B:LYS:H	1:98:B:LEU:HD22	10	0.15
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD21	4	0.15
(1,939)	1:73:B:ILE:H	1:73:B:ILE:HG23	8	0.15
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD11	3	0.15
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB2	4	0.15
(1,812)	1:80:B:THR:HG22	1:81:B:TRP:HZ2	9	0.15
(1,723)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	7	0.15
(1,722)	1:90:B:GLY:HA3	1:30:B:PHE:HE2	8	0.15
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD12	3	0.15
(1,650)	1:43:B:ILE:HG23	1:97:B:HIS:HB3	6	0.15
(1,598)	1:26:B:ILE:HG23	1:90:B:GLY:HA3	9	0.15
(1,589)	1:78:B:ALA:HB1	1:14:B:TRP:HD1	6	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB3	1	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	2	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	3	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	4	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB1	7	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	8	0.15
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	9	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	2	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	4	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	8	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	9	0.15
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	10	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD11	4	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD13	5	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD11	6	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD13	8	0.15
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD11	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:28:B:LYS:HG3	1:28:B:LYS:HA	8	0.15
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	1	0.15
(1,394)	1:99:B:ILE:HG12	1:95:B:GLU:HA	1	0.15
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD13	4	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG23	4	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG21	5	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG21	8	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG22	9	0.15
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG21	10	0.15
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	10	0.15
(1,92)	1:30:B:PHE:HB2	1:40:B:PHE:HB3	4	0.15
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	2	0.15
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD13	10	0.14
(2,1528)	1:32:B:GLN:H	1:31:B:ILE:HG12	9	0.14
(2,1521)	1:56:B:GLU:H	1:55:B:PRO:HB3	5	0.14
(2,1490)	1:35:B:ASP:H	1:36:B:LEU:HB2	2	0.14
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	1	0.14
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	9	0.14
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD12	1	0.14
(2,1436)	1:60:B:LYS:H	1:63:B:ASP:HB3	1	0.14
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	2	0.14
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	7	0.14
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD22	2	0.14
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	5	0.14
(2,1241)	1:87:B:GLU:H	1:89:B:ILE:HB	6	0.14
(2,1158)	1:31:B:ILE:HD13	1:27:B:CYS:HB3	9	0.14
(2,1135)	1:27:B:CYS:H	1:24:B:ASP:HA	7	0.14
(2,1130)	1:83:B:ARG:HD3	1:80:B:THR:HG22	6	0.14
(2,1097)	1:98:B:LEU:HD23	1:39:B:ARG:HA	6	0.14
(2,1095)	1:15:B:LEU:HD12	1:66:B:TYR:H	9	0.14
(2,1084)	1:53:B:LEU:HD12	1:96:B:LYS:HD3	8	0.14
(2,1069)	1:68:B:SER:HB3	1:81:B:TRP:HZ2	1	0.14
(2,1044)	1:95:B:GLU:HB2	1:99:B:ILE:HD13	1	0.14
(2,1031)	1:51:B:VAL:HA	1:23:B:PRO:HA	2	0.14
(2,1031)	1:51:B:VAL:HA	1:23:B:PRO:HA	6	0.14
(2,1031)	1:51:B:VAL:HA	1:23:B:PRO:HA	7	0.14
(2,1018)	1:22:B:LEU:H	1:18:B:MET:HG3	10	0.14
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	4	0.14
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	6	0.14
(2,1013)	1:18:B:MET:HG2	1:15:B:LEU:HA	7	0.14
(2,983)	1:28:B:LYS:HD3	1:32:B:GLN:HG3	1	0.14
(2,971)	1:8:B:GLU:H	1:8:B:GLU:HG2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	1	0.14
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	7	0.14
(2,964)	1:7:B:ASN:HB3	1:8:B:GLU:HG2	1	0.14
(2,947)	1:37:B:LYS:HG3	1:41:B:ASP:HB3	5	0.14
(2,928)	1:65:B:LEU:HB3	1:85:B:LEU:HD12	6	0.14
(2,924)	1:39:B:ARG:HD2	1:43:B:ILE:HG13	7	0.14
(2,914)	1:73:B:ILE:HG13	1:14:B:TRP:HE3	3	0.14
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE1	8	0.14
(2,858)	1:58:B:THR:HG23	1:23:B:PRO:HD2	6	0.14
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	1	0.14
(2,832)	1:8:B:GLU:HG3	1:74:B:ASN:HA	4	0.14
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD2	8	0.14
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD2	9	0.14
(2,815)	1:43:B:ILE:H	1:43:B:ILE:HD12	10	0.14
(2,802)	1:26:B:ILE:HG23	1:86:B:GLY:HA2	7	0.14
(2,783)	1:26:B:ILE:H	1:54:B:ILE:HG22	5	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG22	1	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG22	3	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG22	4	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG23	5	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG21	6	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG21	7	0.14
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG23	10	0.14
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	9	0.14
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	2	0.14
(2,690)	1:11:B:LYS:H	1:11:B:LYS:HA	9	0.14
(2,687)	1:38:B:LYS:HA	1:41:B:ASP:H	7	0.14
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	9	0.14
(2,621)	1:11:B:LYS:HG3	1:69:B:MET:HE1	4	0.14
(2,614)	1:77:B:THR:HB	1:77:B:THR:HG23	3	0.14
(2,614)	1:77:B:THR:HA	1:77:B:THR:HG23	10	0.14
(2,610)	1:54:B:ILE:H	1:50:B:CYS:HA	1	0.14
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	4	0.14
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	6	0.14
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	8	0.14
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	10	0.14
(2,583)	1:21:B:LEU:HD12	1:17:B:SER:HB3	2	0.14
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	2	0.14
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	8	0.14
(2,565)	1:15:B:LEU:HD22	1:62:B:GLN:HA	6	0.14
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	2	0.14
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	2	0.14
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	1	0.14
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	6	0.14
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	7	0.14
(2,455)	1:65:B:LEU:HG	1:65:B:LEU:HB3	9	0.14
(2,411)	1:30:B:PHE:HB2	1:31:B:ILE:HG12	2	0.14
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	3	0.14
(2,399)	1:91:B:LYS:HD3	1:91:B:LYS:HA	9	0.14
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD2	8	0.14
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	6	0.14
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE2	5	0.14
(2,153)	1:56:B:GLU:HG3	1:53:B:LEU:HA	1	0.14
(2,153)	1:76:B:GLU:HG2	1:77:B:THR:HA	5	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG23	1	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	4	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG22	7	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG21	8	0.14
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG23	10	0.14
(2,96)	1:93:B:PHE:HB2	1:54:B:ILE:HG23	2	0.14
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	4	0.14
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	4	0.14
(2,45)	1:61:B:CYS:HB3	1:89:B:ILE:HG13	6	0.14
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	6	0.14
(2,44)	1:61:B:CYS:HB3	1:88:B:CYS:HB2	10	0.14
(1,1305)	1:52:B:THR:H	1:54:B:ILE:HD12	3	0.14
(1,1154)	1:93:B:PHE:H	1:92:B:ASP:HB2	8	0.14
(1,1142)	1:8:B:GLU:H	1:6:B:PRO:HB2	1	0.14
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD11	1	0.14
(1,1104)	1:44:B:LYS:H	1:43:B:ILE:HD13	4	0.14
(1,1041)	1:99:B:ILE:H	1:98:B:LEU:HD23	5	0.14
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	6	0.14
(1,943)	1:87:B:GLU:H	1:85:B:LEU:HD22	1	0.14
(1,831)	1:4:B:ALA:HB1	1:5:B:ASN:HA	9	0.14
(1,771)	1:43:B:ILE:H	1:45:B:MET:HB3	1	0.14
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	9	0.14
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	3	0.14
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	10	0.14
(1,693)	1:89:B:ILE:HB	1:26:B:ILE:HD13	2	0.14
(1,615)	1:43:B:ILE:HD12	1:98:B:LEU:HA	4	0.14
(1,590)	1:78:B:ALA:HB1	1:73:B:ILE:HG23	6	0.14
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	1	0.14
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	5	0.14
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	6	0.14
(1,488)	1:81:B:TRP:HB2	1:81:B:TRP:HA	7	0.14
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD12	1	0.14
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD11	7	0.14
(1,399)	1:55:B:PRO:HG3	1:52:B:THR:HA	9	0.14
(1,398)	1:52:B:THR:HA	1:55:B:PRO:HD3	10	0.14
(1,384)	1:39:B:ARG:HG2	1:98:B:LEU:HD13	1	0.14
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG23	3	0.14
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG22	6	0.14
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	1	0.14
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	5	0.14
(1,187)	1:97:B:HIS:H	1:96:B:LYS:HB3	4	0.14
(1,187)	1:97:B:HIS:H	1:96:B:LYS:HB3	7	0.14
(1,187)	1:97:B:HIS:H	1:96:B:LYS:HB3	8	0.14
(2,1658)	1:77:B:THR:H	1:8:B:GLU:HG3	8	0.13
(2,1605)	1:97:B:HIS:H	1:98:B:LEU:HD22	8	0.13
(2,1574)	1:19:B:THR:H	1:20:B:PRO:HG2	1	0.13
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	2	0.13
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	6	0.13
(2,1511)	1:16:B:ASN:H	1:15:B:LEU:HD11	6	0.13
(2,1466)	1:22:B:LEU:H	1:22:B:LEU:HD23	4	0.13
(2,1439)	1:60:B:LYS:H	1:59:B:LYS:HG3	6	0.13
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	5	0.13
(2,1434)	1:60:B:LYS:H	1:57:B:SER:HB3	4	0.13
(2,1414)	1:41:B:ASP:H	1:42:B:GLU:HG3	8	0.13
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	8	0.13
(2,1376)	1:30:B:PHE:H	1:26:B:ILE:HA	2	0.13
(2,1365)	1:11:B:LYS:H	1:12:B:ASP:HB3	2	0.13
(2,1163)	1:54:B:ILE:HD11	1:23:B:PRO:HG3	4	0.13
(2,1125)	1:48:B:GLU:HG2	1:51:B:VAL:HG21	10	0.13
(2,1124)	1:51:B:VAL:HG11	1:23:B:PRO:HG2	3	0.13
(2,1124)	1:51:B:VAL:HG12	1:23:B:PRO:HG2	4	0.13
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	3	0.13
(2,1115)	1:85:B:LEU:H	1:83:B:ARG:HA	10	0.13
(2,1084)	1:53:B:LEU:HD11	1:96:B:LYS:HD3	10	0.13
(2,1062)	1:57:B:SER:HB3	1:89:B:ILE:HB	2	0.13
(2,996)	1:100:B:PRO:HB2	1:101:B:LYS:HG3	4	0.13
(2,902)	1:81:B:TRP:HB3	1:69:B:MET:HE2	10	0.13
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE3	9	0.13
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	3	0.13
(2,875)	1:90:B:GLY:HA2	1:94:B:ALA:HB1	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,861)	1:70:B:PRO:HD2	1:81:B:TRP:HD1	1	0.13
(2,858)	1:58:B:THR:HG21	1:23:B:PRO:HD2	2	0.13
(2,833)	1:8:B:GLU:HB2	1:74:B:ASN:HA	10	0.13
(2,818)	1:67:B:ALA:HA	1:66:B:TYR:HD1	2	0.13
(2,805)	1:78:B:ALA:HA	1:14:B:TRP:HH2	4	0.13
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG21	6	0.13
(2,789)	1:26:B:ILE:HG12	1:54:B:ILE:HG22	8	0.13
(2,761)	1:13:B:ALA:HB2	1:9:B:MET:HA	4	0.13
(2,756)	1:-1:B:LYS:HD3	1:-1:B:LYS:HA	7	0.13
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG23	2	0.13
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG23	8	0.13
(2,725)	1:80:B:THR:HB	1:80:B:THR:HG21	9	0.13
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	4	0.13
(2,717)	1:65:B:LEU:H	1:64:B:GLU:HA	10	0.13
(2,712)	1:51:B:VAL:HG12	1:47:B:TYR:HE1	3	0.13
(2,709)	1:51:B:VAL:HG23	1:52:B:THR:HA	5	0.13
(2,687)	1:94:B:ALA:H	1:91:B:LYS:HA	9	0.13
(2,683)	1:87:B:GLU:H	1:83:B:ARG:HA	1	0.13
(2,673)	1:69:B:MET:HB3	1:11:B:LYS:HA	4	0.13
(2,640)	1:-6:B:VAL:HA	1:-7:B:HIS:HA	4	0.13
(2,614)	1:77:B:THR:HA	1:77:B:THR:HG22	8	0.13
(2,608)	1:85:B:LEU:HD23	1:62:B:GLN:HB2	1	0.13
(2,608)	1:85:B:LEU:HD22	1:62:B:GLN:HB2	9	0.13
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	1	0.13
(2,588)	1:84:B:SER:HB3	1:84:B:SER:HA	7	0.13
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	3	0.13
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE2	1	0.13
(2,558)	1:36:B:LEU:H	1:36:B:LEU:HD22	8	0.13
(2,558)	1:36:B:LEU:H	1:36:B:LEU:HD21	9	0.13
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	7	0.13
(2,489)	1:100:B:PRO:HG2	1:101:B:LYS:HE3	7	0.13
(2,485)	1:92:B:ASP:HB3	1:57:B:SER:HB2	6	0.13
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	6	0.13
(2,471)	1:39:B:ARG:HG3	1:39:B:ARG:HA	2	0.13
(2,365)	1:33:B:ASP:H	1:32:B:GLN:HB3	3	0.13
(2,345)	1:91:B:LYS:H	1:91:B:LYS:HD2	8	0.13
(2,303)	1:61:B:CYS:H	1:60:B:LYS:HD2	7	0.13
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	9	0.13
(2,214)	1:28:B:LYS:H	1:28:B:LYS:HB3	3	0.13
(2,168)	1:54:B:ILE:HB	1:51:B:VAL:HG13	6	0.13
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	8	0.13
(2,133)	1:31:B:ILE:HB	1:31:B:ILE:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	10	0.13
(2,122)	1:15:B:LEU:H	1:16:B:ASN:HB2	8	0.13
(2,116)	1:89:B:ILE:HB	1:26:B:ILE:HG21	3	0.13
(2,101)	1:63:B:ASP:HB2	1:60:B:LYS:HA	9	0.13
(2,91)	1:90:B:GLY:H	1:93:B:PHE:HB3	2	0.13
(2,75)	1:36:B:LEU:HB3	1:37:B:LYS:HA	3	0.13
(2,60)	1:85:B:LEU:HB2	1:14:B:TRP:HH2	8	0.13
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	7	0.13
(2,47)	1:85:B:LEU:HB3	1:89:B:ILE:H	10	0.13
(2,42)	1:89:B:ILE:H	1:61:B:CYS:HB3	6	0.13
(2,38)	1:60:B:LYS:HE2	1:60:B:LYS:HB2	4	0.13
(2,25)	1:33:B:ASP:HB3	1:34:B:PRO:HD2	2	0.13
(2,12)	1:83:B:ARG:HD2	1:83:B:ARG:HG2	2	0.13
(1,1318)	1:43:B:ILE:H	1:39:B:ARG:HG2	6	0.13
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD13	8	0.13
(1,1168)	1:12:B:ASP:H	1:15:B:LEU:HD12	7	0.13
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB2	4	0.13
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	10	0.13
(1,1130)	1:39:B:ARG:H	1:38:B:LYS:HG2	5	0.13
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	3	0.13
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD23	2	0.13
(1,833)	1:99:B:ILE:H	1:94:B:ALA:HB3	5	0.13
(1,825)	1:93:B:PHE:H	1:89:B:ILE:HG23	3	0.13
(1,810)	1:19:B:THR:H	1:19:B:THR:HG21	8	0.13
(1,785)	1:57:B:SER:HB3	1:93:B:PHE:H	2	0.13
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG21	4	0.13
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	6	0.13
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	7	0.13
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	10	0.13
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	1	0.13
(1,653)	1:31:B:ILE:HD13	1:47:B:TYR:HA	1	0.13
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG21	2	0.13
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG22	10	0.13
(1,631)	1:43:B:ILE:HD13	1:100:B:PRO:HD3	5	0.13
(1,631)	1:43:B:ILE:HD11	1:100:B:PRO:HD3	10	0.13
(1,590)	1:78:B:ALA:HB1	1:73:B:ILE:HG23	4	0.13
(1,480)	1:98:B:LEU:HD21	1:97:B:HIS:HB3	1	0.13
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE2	9	0.13
(1,477)	1:98:B:LEU:HD21	1:93:B:PHE:HE2	10	0.13
(1,415)	1:65:B:LEU:HG	1:65:B:LEU:HD13	3	0.13
(1,379)	1:57:B:SER:HB2	1:54:B:ILE:HD12	5	0.13
(2,1581)	1:24:B:ASP:H	1:54:B:ILE:HG23	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1578)	1:19:B:THR:H	1:22:B:LEU:HD11	1	0.12
(2,1543)	1:84:B:SER:H	1:81:B:TRP:HE3	9	0.12
(2,1540)	1:72:B:LYS:H	1:72:B:LYS:HG2	5	0.12
(2,1531)	1:98:B:LEU:H	1:43:B:ILE:HD11	7	0.12
(2,1521)	1:56:B:GLU:H	1:55:B:PRO:HB3	9	0.12
(2,1479)	1:51:B:VAL:H	1:54:B:ILE:HD12	4	0.12
(2,1453)	1:93:B:PHE:H	1:91:B:LYS:HB2	4	0.12
(2,1453)	1:93:B:PHE:H	1:91:B:LYS:HB2	9	0.12
(2,1438)	1:22:B:LEU:H	1:21:B:LEU:HB3	7	0.12
(2,1392)	1:88:B:CYS:H	1:89:B:ILE:HG12	1	0.12
(2,1374)	1:18:B:MET:H	1:15:B:LEU:HD23	5	0.12
(2,1357)	1:58:B:THR:H	1:55:B:PRO:HA	3	0.12
(2,1302)	1:54:B:ILE:H	1:89:B:ILE:HG22	6	0.12
(2,1154)	1:99:B:ILE:HG21	1:101:B:LYS:HA	2	0.12
(2,1124)	1:51:B:VAL:HG13	1:23:B:PRO:HG2	1	0.12
(2,1117)	1:-6:B:VAL:HG12	1:-4:B:ASP:H	1	0.12
(2,1117)	1:-6:B:VAL:HG12	1:-4:B:ASP:H	9	0.12
(2,1098)	1:98:B:LEU:HD22	1:39:B:ARG:HA	1	0.12
(2,1095)	1:12:B:ASP:H	1:15:B:LEU:HD11	6	0.12
(2,1088)	1:60:B:LYS:HG2	1:57:B:SER:HA	5	0.12
(2,1083)	1:45:B:MET:HG2	1:53:B:LEU:HD11	2	0.12
(2,1067)	1:25:B:LEU:H	1:25:B:LEU:HG	8	0.12
(2,1058)	1:44:B:LYS:HD3	1:41:B:ASP:HB3	5	0.12
(2,1034)	1:23:B:PRO:HA	1:54:B:ILE:HD13	2	0.12
(2,968)	1:9:B:MET:HB3	1:14:B:TRP:HB2	4	0.12
(2,967)	1:64:B:GLU:HG3	1:63:B:ASP:HB3	1	0.12
(2,939)	1:35:B:ASP:HB2	1:36:B:LEU:HB2	9	0.12
(2,900)	1:11:B:LYS:HB3	1:69:B:MET:HE3	10	0.12
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	5	0.12
(2,883)	1:90:B:GLY:HA3	1:89:B:ILE:HB	9	0.12
(2,874)	1:26:B:ILE:HD12	1:90:B:GLY:HA3	5	0.12
(2,873)	1:26:B:ILE:HD12	1:90:B:GLY:HA2	7	0.12
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	2	0.12
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	3	0.12
(2,717)	1:84:B:SER:H	1:83:B:ARG:HA	8	0.12
(2,713)	1:51:B:VAL:HG13	1:24:B:ASP:HA	1	0.12
(2,709)	1:51:B:VAL:HG22	1:52:B:THR:HA	4	0.12
(2,709)	1:51:B:VAL:HG23	1:52:B:THR:HA	7	0.12
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	7	0.12
(2,603)	1:75:B:SER:HA	1:78:B:ALA:HB2	3	0.12
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	3	0.12
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	8	0.12
(2,552)	1:64:B:GLU:HG2	1:60:B:LYS:HG3	10	0.12
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	9	0.12
(2,402)	1:54:B:ILE:H	1:54:B:ILE:HG13	9	0.12
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD2	10	0.12
(2,330)	1:39:B:ARG:HB3	1:98:B:LEU:HD22	1	0.12
(2,292)	1:64:B:GLU:HB2	1:65:B:LEU:HD11	6	0.12
(2,257)	1:23:B:PRO:HB3	1:24:B:ASP:H	3	0.12
(2,238)	1:9:B:MET:HG2	1:10:B:THR:HA	6	0.12
(2,214)	1:28:B:LYS:H	1:28:B:LYS:HB3	8	0.12
(2,214)	1:28:B:LYS:H	1:28:B:LYS:HB3	9	0.12
(2,214)	1:28:B:LYS:H	1:28:B:LYS:HB3	10	0.12
(2,188)	1:0:B:MET:HB2	1:-1:B:LYS:H	6	0.12
(2,175)	1:46:B:THR:H	1:49:B:GLN:HG2	6	0.12
(2,75)	1:36:B:LEU:HB3	1:37:B:LYS:HA	9	0.12
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	1	0.12
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	2	0.12
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	8	0.12
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	1	0.12
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	2	0.12
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	8	0.12
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB3	6	0.12
(2,12)	1:83:B:ARG:HD3	1:83:B:ARG:HG2	8	0.12
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD13	7	0.12
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD11	8	0.12
(1,1199)	1:48:B:GLU:H	1:31:B:ILE:HD11	10	0.12
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB3	1	0.12
(1,1152)	1:93:B:PHE:H	1:90:B:GLY:HA3	6	0.12
(1,1130)	1:39:B:ARG:H	1:38:B:LYS:HG2	1	0.12
(1,1035)	1:42:B:GLU:H	1:41:B:ASP:HB2	9	0.12
(1,967)	1:54:B:ILE:H	1:53:B:LEU:HD22	6	0.12
(1,942)	1:87:B:GLU:H	1:65:B:LEU:HD13	2	0.12
(1,877)	1:74:B:ASN:H	1:73:B:ILE:HG22	3	0.12
(1,846)	1:96:B:LYS:HB2	1:97:B:HIS:HA	3	0.12
(1,835)	1:86:B:GLY:H	1:89:B:ILE:HD13	4	0.12
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB1	2	0.12
(1,825)	1:93:B:PHE:H	1:89:B:ILE:HG23	2	0.12
(1,825)	1:93:B:PHE:H	1:89:B:ILE:HG23	5	0.12
(1,808)	1:53:B:LEU:HA	1:52:B:THR:HG22	4	0.12
(1,753)	1:54:B:ILE:HA	1:53:B:LEU:HB3	10	0.12
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG23	1	0.12
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG23	5	0.12
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG21	8	0.12
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	10	0.12
(1,740)	1:11:B:LYS:HB3	1:11:B:LYS:HE2	5	0.12
(1,704)	1:91:B:LYS:H	1:90:B:GLY:HA2	9	0.12
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	4	0.12
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	8	0.12
(1,699)	1:82:B:GLY:HA3	1:14:B:TRP:HH2	9	0.12
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	3	0.12
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	5	0.12
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	6	0.12
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	7	0.12
(1,674)	1:5:B:ASN:HA	1:5:B:ASN:HB2	8	0.12
(1,650)	1:43:B:ILE:HG23	1:97:B:HIS:HB3	7	0.12
(1,631)	1:43:B:ILE:HD12	1:100:B:PRO:HD3	3	0.12
(1,582)	1:94:B:ALA:HB1	1:94:B:ALA:HA	4	0.12
(1,582)	1:94:B:ALA:HB2	1:94:B:ALA:HA	9	0.12
(1,580)	1:94:B:ALA:HB2	1:30:B:PHE:HZ	3	0.12
(1,559)	1:66:B:TYR:HB2	1:63:B:ASP:HA	2	0.12
(1,475)	1:98:B:LEU:H	1:98:B:LEU:HD23	7	0.12
(1,467)	1:74:B:ASN:H	1:77:B:THR:HG21	3	0.12
(1,455)	1:85:B:LEU:HD21	1:85:B:LEU:H	7	0.12
(1,408)	1:28:B:LYS:HG3	1:28:B:LYS:H	7	0.12
(1,406)	1:53:B:LEU:HG	1:53:B:LEU:HA	8	0.12
(1,405)	1:18:B:MET:HG2	1:85:B:LEU:HD11	7	0.12
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	9	0.12
(1,325)	1:81:B:TRP:HB3	1:81:B:TRP:HD1	2	0.12
(1,325)	1:81:B:TRP:HB3	1:81:B:TRP:HD1	6	0.12
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG22	7	0.12
(1,200)	1:97:B:HIS:HB2	1:45:B:MET:HE1	7	0.12
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	9	0.12
(2,1631)	1:29:B:GLY:H	1:31:B:ILE:HD12	9	0.11
(2,1562)	1:21:B:LEU:H	1:58:B:THR:HG23	4	0.11
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	4	0.11
(2,1458)	1:93:B:PHE:H	1:54:B:ILE:HD12	2	0.11
(2,1453)	1:93:B:PHE:H	1:91:B:LYS:HB2	3	0.11
(2,1420)	1:41:B:ASP:H	1:39:B:ARG:HG3	3	0.11
(2,1396)	1:49:B:GLN:H	1:47:B:TYR:HB2	6	0.11
(2,1294)	1:14:B:TRP:H	1:11:B:LYS:HB3	9	0.11
(2,1270)	1:54:B:ILE:H	1:51:B:VAL:HG12	7	0.11
(2,1240)	1:87:B:GLU:H	1:83:B:ARG:HB2	1	0.11
(2,1240)	1:87:B:GLU:H	1:83:B:ARG:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1210)	1:33:B:ASP:H	1:36:B:LEU:HB3	5	0.11
(2,1209)	1:33:B:ASP:H	1:37:B:LYS:HG2	4	0.11
(2,1097)	1:98:B:LEU:HD22	1:39:B:ARG:HA	3	0.11
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD11	3	0.11
(2,1054)	1:26:B:ILE:HG13	1:90:B:GLY:HA2	5	0.11
(2,1018)	1:22:B:LEU:H	1:18:B:MET:HG3	4	0.11
(2,944)	1:93:B:PHE:HB2	1:96:B:LYS:HD2	1	0.11
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	1	0.11
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	5	0.11
(2,925)	1:83:B:ARG:H	1:83:B:ARG:HD2	4	0.11
(2,910)	1:31:B:ILE:HD13	1:40:B:PHE:HE1	4	0.11
(2,897)	1:69:B:MET:HE2	1:11:B:LYS:HE2	3	0.11
(2,848)	1:39:B:ARG:HD2	1:100:B:PRO:HD2	3	0.11
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	3	0.11
(2,793)	1:57:B:SER:H	1:89:B:ILE:HG23	6	0.11
(2,785)	1:54:B:ILE:HG22	1:23:B:PRO:HD3	3	0.11
(2,769)	1:21:B:LEU:HB2	1:18:B:MET:HA	9	0.11
(2,765)	1:77:B:THR:HB	1:78:B:ALA:HB2	5	0.11
(2,720)	1:25:B:LEU:HB2	1:22:B:LEU:HA	3	0.11
(2,719)	1:64:B:GLU:HA	1:64:B:GLU:HG2	5	0.11
(2,708)	1:24:B:ASP:H	1:51:B:VAL:HG11	5	0.11
(2,708)	1:24:B:ASP:H	1:51:B:VAL:HG12	7	0.11
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	4	0.11
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	8	0.11
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	10	0.11
(2,588)	1:17:B:SER:HB3	1:17:B:SER:HA	2	0.11
(2,568)	1:47:B:TYR:HA	1:40:B:PHE:HE2	4	0.11
(2,543)	1:54:B:ILE:HA	1:53:B:LEU:HB3	2	0.11
(2,494)	1:83:B:ARG:HG3	1:87:B:GLU:HG2	7	0.11
(2,481)	1:86:B:GLY:H	1:85:B:LEU:HG	8	0.11
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	7	0.11
(2,478)	1:15:B:LEU:HG	1:12:B:ASP:HA	10	0.11
(2,373)	1:101:B:LYS:H	1:101:B:LYS:HD2	5	0.11
(2,353)	1:49:B:GLN:HB3	1:45:B:MET:HA	10	0.11
(2,289)	1:42:B:GLU:HB2	1:43:B:ILE:HG13	2	0.11
(2,274)	1:22:B:LEU:H	1:19:B:THR:HA	8	0.11
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	7	0.11
(2,238)	1:9:B:MET:HG2	1:8:B:GLU:HA	3	0.11
(2,192)	1:91:B:LYS:H	1:91:B:LYS:HB2	8	0.11
(2,162)	1:72:B:LYS:HB3	1:72:B:LYS:HE2	4	0.11
(2,153)	1:76:B:GLU:HG2	1:77:B:THR:HA	8	0.11
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	4	0.11
(2,75)	1:36:B:LEU:HB3	1:37:B:LYS:HA	8	0.11
(2,75)	1:36:B:LEU:HB3	1:37:B:LYS:HA	10	0.11
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	3	0.11
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	3	0.11
(2,49)	1:21:B:LEU:HB2	1:21:B:LEU:HA	1	0.11
(2,49)	1:21:B:LEU:HB2	1:21:B:LEU:HA	10	0.11
(2,36)	1:61:B:CYS:HB2	1:58:B:THR:HA	5	0.11
(2,35)	1:37:B:LYS:HE2	1:41:B:ASP:H	5	0.11
(2,17)	1:92:B:ASP:HB3	1:57:B:SER:HA	1	0.11
(2,14)	1:91:B:LYS:H	1:92:B:ASP:HB2	9	0.11
(2,12)	1:83:B:ARG:HD3	1:83:B:ARG:HG2	3	0.11
(2,12)	1:83:B:ARG:HD3	1:83:B:ARG:HG2	5	0.11
(2,12)	1:83:B:ARG:HD3	1:83:B:ARG:HG2	7	0.11
(2,11)	1:39:B:ARG:HD2	1:39:B:ARG:HG3	4	0.11
(2,8)	1:35:B:ASP:H	1:33:B:ASP:HB2	1	0.11
(2,4)	1:53:B:LEU:HB2	1:49:B:GLN:HG3	4	0.11
(1,1241)	1:21:B:LEU:H	1:21:B:LEU:HD11	3	0.11
(1,1167)	1:12:B:ASP:H	1:13:B:ALA:HB1	7	0.11
(1,1130)	1:39:B:ARG:H	1:38:B:LYS:HG2	4	0.11
(1,1130)	1:39:B:ARG:H	1:38:B:LYS:HG2	8	0.11
(1,1121)	1:44:B:LYS:H	1:98:B:LEU:HD22	8	0.11
(1,877)	1:74:B:ASN:H	1:73:B:ILE:HG21	1	0.11
(1,846)	1:96:B:LYS:HB2	1:97:B:HIS:HA	7	0.11
(1,832)	1:96:B:LYS:H	1:94:B:ALA:HB3	7	0.11
(1,768)	1:97:B:HIS:HB2	1:96:B:LYS:HB3	4	0.11
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	1	0.11
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG21	2	0.11
(1,764)	1:54:B:ILE:HB	1:89:B:ILE:HG23	10	0.11
(1,761)	1:66:B:TYR:HB3	1:15:B:LEU:HD12	8	0.11
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	2	0.11
(1,752)	1:10:B:THR:HB	1:10:B:THR:HG22	9	0.11
(1,690)	1:26:B:ILE:HD11	1:30:B:PHE:HE2	1	0.11
(1,653)	1:31:B:ILE:HD13	1:47:B:TYR:HA	6	0.11
(1,653)	1:31:B:ILE:HD13	1:47:B:TYR:HA	9	0.11
(1,612)	1:78:B:ALA:HB2	1:78:B:ALA:HA	5	0.11
(1,612)	1:78:B:ALA:HB1	1:78:B:ALA:HA	9	0.11
(1,590)	1:78:B:ALA:HB2	1:73:B:ILE:HG23	10	0.11
(1,582)	1:94:B:ALA:HB2	1:94:B:ALA:HA	1	0.11
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	3	0.11
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	5	0.11
(1,582)	1:94:B:ALA:HB1	1:94:B:ALA:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	8	0.11
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	10	0.11
(1,578)	1:94:B:ALA:H	1:94:B:ALA:HB2	5	0.11
(1,508)	1:10:B:THR:H	1:10:B:THR:HG23	8	0.11
(1,477)	1:98:B:LEU:HD23	1:93:B:PHE:HE2	1	0.11
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE1	2	0.11
(1,477)	1:98:B:LEU:HD22	1:93:B:PHE:HE1	5	0.11
(1,463)	1:96:B:LYS:HB3	1:93:B:PHE:HA	3	0.11
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	1	0.11
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD11	2	0.11
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	7	0.11
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD11	9	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	1	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	2	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	3	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	6	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	7	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	8	0.11
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	10	0.11
(1,406)	1:53:B:LEU:HG	1:53:B:LEU:HA	9	0.11
(1,400)	1:28:B:LYS:HG3	1:28:B:LYS:HA	7	0.11
(1,380)	1:81:B:TRP:HE1	1:70:B:PRO:HG2	10	0.11
(1,325)	1:81:B:TRP:HB3	1:81:B:TRP:HD1	1	0.11
(1,237)	1:77:B:THR:HB	1:77:B:THR:HG21	2	0.11
(1,222)	1:45:B:MET:HB2	1:98:B:LEU:HD22	8	0.11
(1,203)	1:97:B:HIS:HB2	1:93:B:PHE:HD1	6	0.11
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	2	0.11
(1,191)	1:96:B:LYS:HB2	1:96:B:LYS:HA	6	0.11
(1,93)	1:30:B:PHE:HB2	1:36:B:LEU:HB3	8	0.11
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	9	0.11
(2,1574)	1:19:B:THR:H	1:20:B:PRO:HG2	2	0.1
(2,1532)	1:98:B:LEU:H	1:98:B:LEU:HD11	9	0.1
(2,1480)	1:51:B:VAL:H	1:47:B:TYR:HA	10	0.1
(2,1427)	1:44:B:LYS:H	1:43:B:ILE:HG12	6	0.1
(2,1376)	1:30:B:PHE:H	1:26:B:ILE:HA	9	0.1
(2,1242)	1:87:B:GLU:H	1:83:B:ARG:HG2	1	0.1
(2,1137)	1:24:B:ASP:HA	1:28:B:LYS:HG3	1	0.1
(2,1117)	1:-6:B:VAL:HG22	1:-4:B:ASP:H	5	0.1
(2,1079)	1:82:B:GLY:H	1:85:B:LEU:HD12	2	0.1
(2,945)	1:67:B:ALA:HB1	1:66:B:TYR:HB3	3	0.1
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	2	0.1
(2,938)	1:24:B:ASP:HB2	1:23:B:PRO:HB2	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,836)	1:21:B:LEU:HG	1:20:B:PRO:HD2	6	0.1
(2,771)	1:18:B:MET:HG2	1:18:B:MET:HA	3	0.1
(2,771)	1:18:B:MET:HG2	1:18:B:MET:HA	10	0.1
(2,769)	1:21:B:LEU:HB2	1:18:B:MET:HA	3	0.1
(2,699)	1:87:B:GLU:H	1:87:B:GLU:HA	1	0.1
(2,606)	1:85:B:LEU:HD21	1:66:B:TYR:H	3	0.1
(2,593)	1:15:B:LEU:HD21	1:62:B:GLN:HA	10	0.1
(2,577)	1:31:B:ILE:HA	1:37:B:LYS:HG2	9	0.1
(2,430)	1:37:B:LYS:HD2	1:31:B:ILE:HG23	3	0.1
(2,393)	1:48:B:GLU:HB2	1:47:B:TYR:HD1	5	0.1
(2,340)	1:38:B:LYS:H	1:38:B:LYS:HD2	5	0.1
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	1	0.1
(2,262)	1:45:B:MET:HG2	1:50:B:CYS:HA	3	0.1
(2,158)	1:25:B:LEU:H	1:26:B:ILE:HB	5	0.1
(2,135)	1:9:B:MET:HB2	1:14:B:TRP:HD1	9	0.1
(2,128)	1:88:B:CYS:HB2	1:84:B:SER:HA	9	0.1
(2,59)	1:84:B:SER:H	1:85:B:LEU:HB2	10	0.1
(2,56)	1:84:B:SER:H	1:85:B:LEU:HB2	10	0.1
(2,50)	1:21:B:LEU:HB3	1:22:B:LEU:HA	1	0.1
(1,846)	1:96:B:LYS:HB2	1:97:B:HIS:HA	4	0.1
(1,824)	1:99:B:ILE:HG21	1:101:B:LYS:HA	3	0.1
(1,747)	1:37:B:LYS:HB2	1:34:B:PRO:HA	3	0.1
(1,644)	1:77:B:THR:H	1:73:B:ILE:HG23	4	0.1
(1,612)	1:78:B:ALA:HB3	1:78:B:ALA:HA	2	0.1
(1,612)	1:78:B:ALA:HB3	1:78:B:ALA:HA	3	0.1
(1,612)	1:78:B:ALA:HB1	1:78:B:ALA:HA	4	0.1
(1,612)	1:78:B:ALA:HB1	1:78:B:ALA:HA	6	0.1
(1,612)	1:78:B:ALA:HB2	1:78:B:ALA:HA	7	0.1
(1,612)	1:78:B:ALA:HB3	1:78:B:ALA:HA	8	0.1
(1,582)	1:94:B:ALA:HB3	1:94:B:ALA:HA	2	0.1
(1,582)	1:94:B:ALA:HB2	1:94:B:ALA:HA	7	0.1
(1,548)	1:49:B:GLN:HA	1:52:B:THR:HG21	7	0.1
(1,489)	1:64:B:GLU:HB3	1:61:B:CYS:HA	3	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD12	3	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	4	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	5	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD13	8	0.1
(1,441)	1:21:B:LEU:HG	1:21:B:LEU:HD12	10	0.1
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	5	0.1
(1,430)	1:47:B:TYR:HB3	1:47:B:TYR:HA	9	0.1
(1,406)	1:53:B:LEU:HG	1:53:B:LEU:HA	5	0.1
(1,60)	1:36:B:LEU:HB2	1:36:B:LEU:HD21	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:86:B:GLY:H	1:85:B:LEU:HB3	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found