



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 AM UTC

PDB ID : 2LY8 / pdb_00002ly8
BMRB ID : 18713
Title : The budding yeast chaperone Scm3 recognizes the partially unfolded dimer of the centromere-specific Cse4/H4 histone variant
Authors : Hong, J.; Feng, H.; Zhou, Z.; Ghirlando, R.; Bai, Y.
Deposited on : 2012-09-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

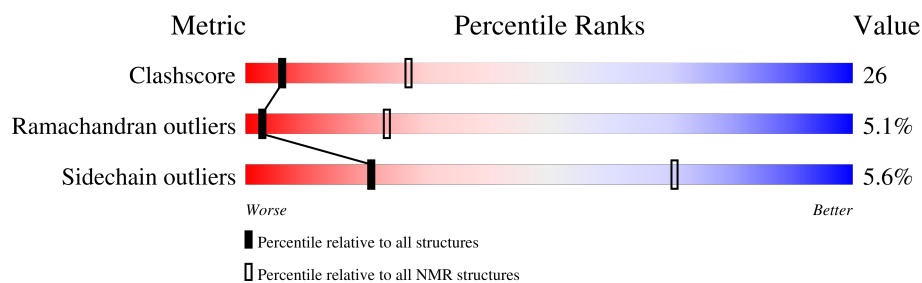
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	121	39% 15% . 42%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:41, A:75-A:109 (70)	0.18	10

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1971 atoms, of which 1005 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Budding yeast chaperone Scm3.

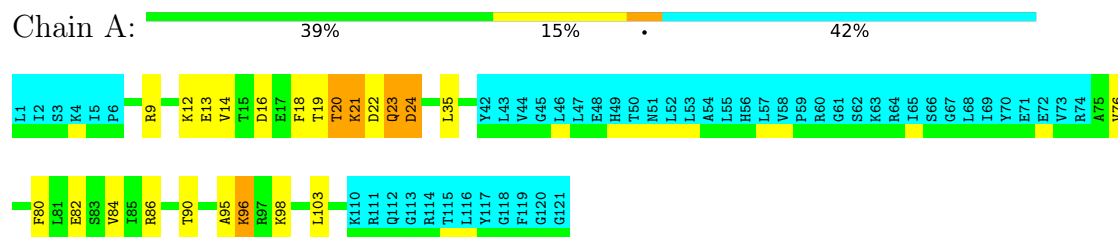
Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1971	618	1005	168	178	2	

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: Budding yeast chaperone Scm3

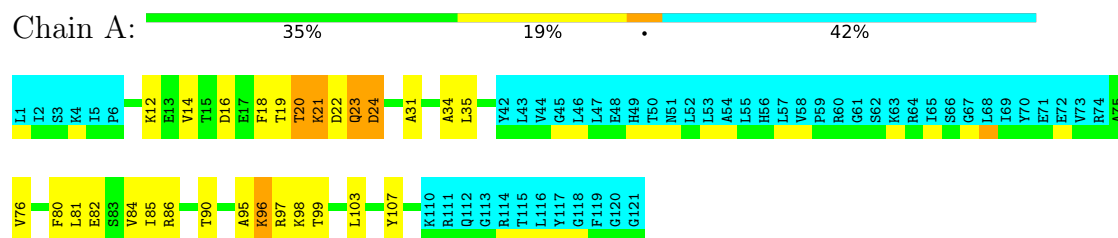


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

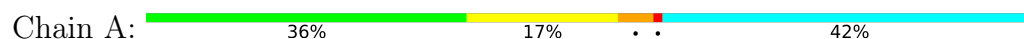
4.2.1 Score per residue for model 1

- Molecule 1: Budding yeast chaperone Scm3



4.2.2 Score per residue for model 2

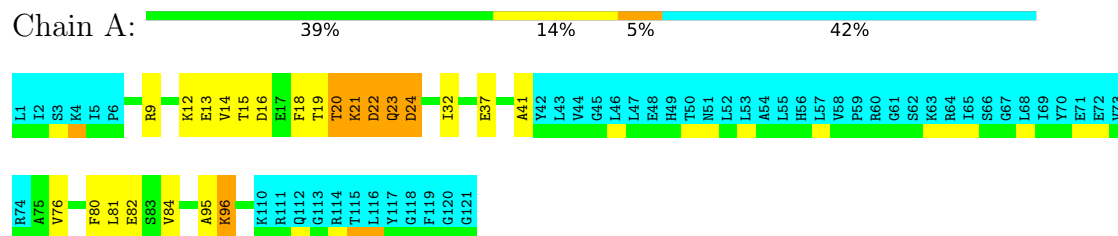
- Molecule 1: Budding yeast chaperone Scm3





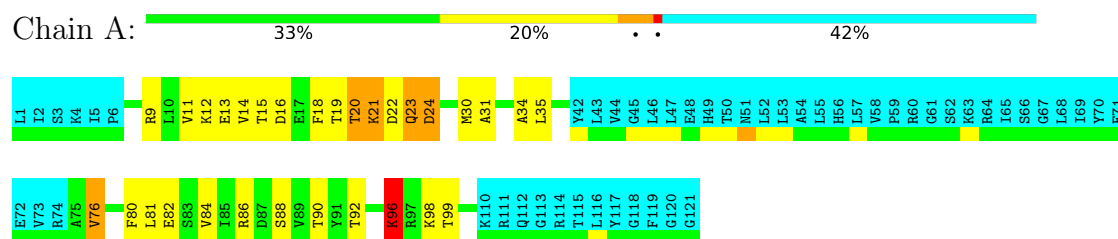
4.2.3 Score per residue for model 3

- Molecule 1: Budding yeast chaperone Scm3



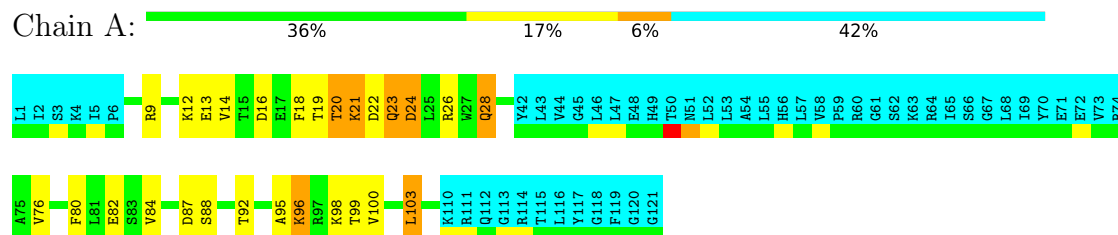
4.2.4 Score per residue for model 4

- Molecule 1: Budding yeast chaperone Scm3



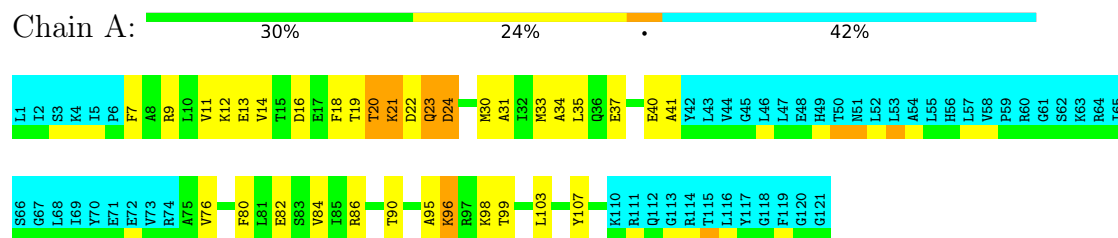
4.2.5 Score per residue for model 5

- Molecule 1: Budding yeast chaperone Scm3



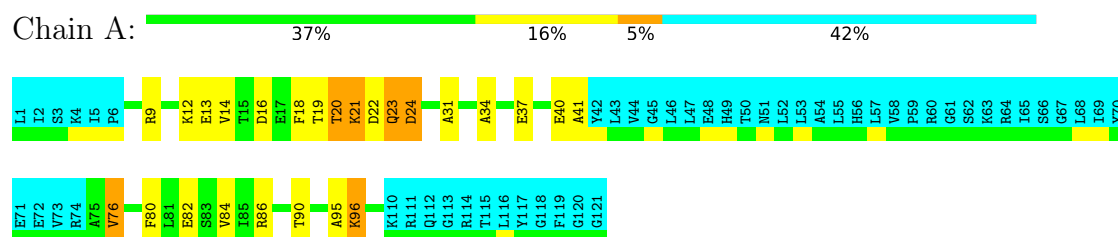
4.2.6 Score per residue for model 6

- Molecule 1: Budding yeast chaperone Scm3



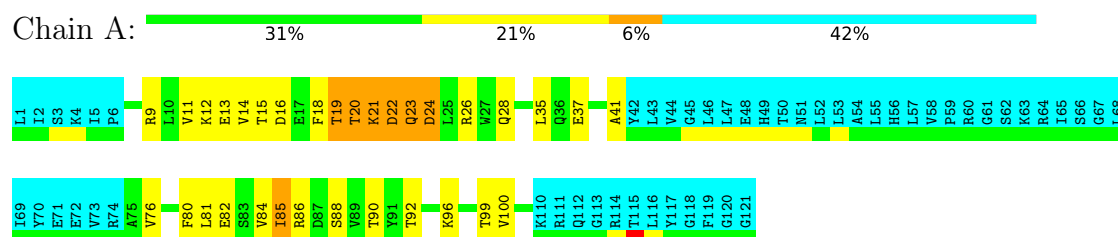
4.2.7 Score per residue for model 7

- Molecule 1: Budding yeast chaperone Scm3



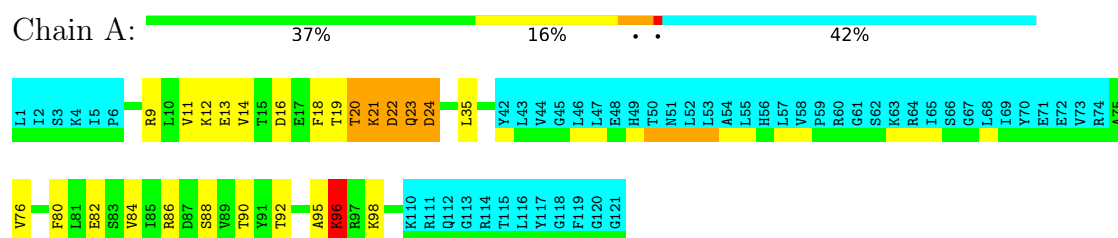
4.2.8 Score per residue for model 8

- Molecule 1: Budding yeast chaperone Scm3



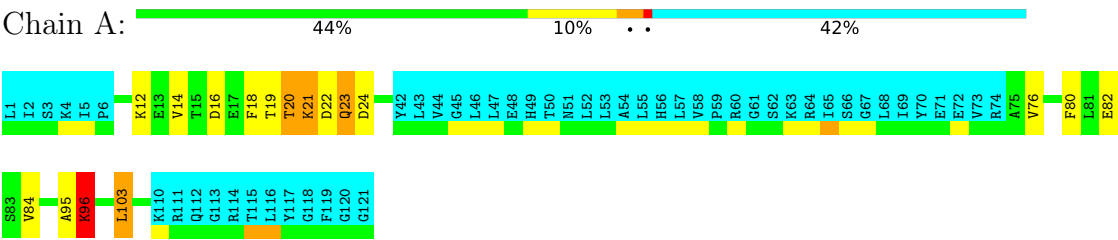
4.2.9 Score per residue for model 9

- Molecule 1: Budding yeast chaperone Scm3



4.2.10 Score per residue for model 10 (medoid)

● Molecule 1: Budding yeast chaperone Scm3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 30 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	updated
ProcheckNMR	structure solution	updated
MOLMOL	structure solution	
X-PLOR NIH	refinement	

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	1446
Number of shifts mapped to atoms	1446
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	560	567	567	30±4
All	All	5600	5670	5670	296

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:PHE:O	1:A:84:VAL:HG23	0.78	1.79	5	10
1:A:28:GLN:N	1:A:28:GLN:CD	0.77	2.42	8	1
1:A:88:SER:O	1:A:92:THR:HG23	0.72	1.84	9	5
1:A:31:ALA:O	1:A:34:ALA:HB3	0.69	1.87	4	5
1:A:15:THR:HG22	1:A:81:LEU:HD13	0.69	1.63	4	2
1:A:15:THR:CG2	1:A:81:LEU:HD13	0.66	2.21	8	2
1:A:19:THR:C	1:A:21:LYS:N	0.61	2.56	8	10
1:A:28:GLN:NE2	1:A:28:GLN:H	0.60	1.93	5	1
1:A:21:LYS:O	1:A:23:GLN:NE2	0.59	2.35	2	10
1:A:28:GLN:NE2	1:A:100:VAL:O	0.58	2.37	5	1
1:A:19:THR:O	1:A:21:LYS:N	0.58	2.37	3	10
1:A:80:PHE:CZ	1:A:84:VAL:HG21	0.57	2.35	4	10
1:A:20:THR:C	1:A:22:ASP:H	0.56	2.08	1	10
1:A:21:LYS:C	1:A:23:GLN:H	0.56	2.08	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:THR:C	1:A:21:LYS:H	0.55	2.10	8	10
1:A:80:PHE:CE1	1:A:84:VAL:CG2	0.54	2.89	7	10
1:A:26:ARG:O	1:A:28:GLN:NE2	0.54	2.40	5	1
1:A:18:PHE:CG	1:A:82:GLU:OE2	0.54	2.61	4	10
1:A:28:GLN:H	1:A:28:GLN:CD	0.54	2.08	5	1
1:A:28:GLN:OE1	1:A:100:VAL:O	0.53	2.27	5	2
1:A:28:GLN:N	1:A:28:GLN:OE1	0.52	2.40	8	1
1:A:18:PHE:CD1	1:A:82:GLU:OE2	0.52	2.62	8	7
1:A:19:THR:OG1	1:A:85:ILE:CD1	0.52	2.58	8	1
1:A:81:LEU:O	1:A:85:ILE:HG12	0.51	2.05	1	1
1:A:92:THR:HG21	1:A:99:THR:O	0.51	2.05	4	1
1:A:16:ASP:O	1:A:20:THR:N	0.50	2.45	6	10
1:A:26:ARG:C	1:A:28:GLN:HE22	0.50	2.14	8	1
1:A:86:ARG:O	1:A:90:THR:OG1	0.49	2.27	9	7
1:A:28:GLN:NE2	1:A:99:THR:HG23	0.49	2.23	8	1
1:A:30:MET:O	1:A:33:MET:HG2	0.49	2.08	6	1
1:A:21:LYS:O	1:A:23:GLN:CD	0.48	2.56	10	2
1:A:103:LEU:O	1:A:107:TYR:CD1	0.48	2.66	1	2
1:A:35:LEU:N	1:A:35:LEU:CD1	0.48	2.77	4	3
1:A:21:LYS:O	1:A:23:GLN:N	0.47	2.46	9	7
1:A:25:LEU:HD12	1:A:25:LEU:N	0.47	2.24	2	1
1:A:18:PHE:CD1	1:A:18:PHE:N	0.47	2.82	1	5
1:A:28:GLN:CD	1:A:28:GLN:N	0.47	2.73	5	1
1:A:18:PHE:N	1:A:18:PHE:CD1	0.47	2.82	4	1
1:A:12:LYS:O	1:A:16:ASP:CG	0.46	2.59	8	10
1:A:21:LYS:C	1:A:23:GLN:N	0.46	2.73	3	10
1:A:95:ALA:O	1:A:97:ARG:N	0.46	2.48	1	1
1:A:95:ALA:O	1:A:96:LYS:CD	0.46	2.64	3	6
1:A:9:ARG:O	1:A:13:GLU:CG	0.46	2.63	6	7
1:A:103:LEU:HD13	1:A:103:LEU:O	0.46	2.10	2	3
1:A:20:THR:C	1:A:22:ASP:N	0.46	2.73	1	10
1:A:7:PHE:C	1:A:7:PHE:CD1	0.46	2.93	6	1
1:A:7:PHE:CE1	1:A:11:VAL:HG21	0.46	2.45	6	1
1:A:92:THR:O	1:A:96:LYS:N	0.46	2.48	4	1
1:A:11:VAL:HG13	1:A:12:LYS:N	0.46	2.26	9	2
1:A:23:GLN:O	1:A:24:ASP:OD1	0.46	2.34	7	10
1:A:35:LEU:N	1:A:35:LEU:HD12	0.46	2.24	4	1
1:A:28:GLN:NE2	1:A:28:GLN:N	0.46	2.64	5	1
1:A:11:VAL:O	1:A:15:THR:HG23	0.45	2.11	4	1
1:A:14:VAL:CG1	1:A:18:PHE:CZ	0.45	3.00	10	10
1:A:28:GLN:HE22	1:A:100:VAL:N	0.45	2.09	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLN:CD	1:A:99:THR:HG23	0.45	2.37	8	1
1:A:19:THR:OG1	1:A:85:ILE:HD12	0.45	2.12	1	1
1:A:35:LEU:HD12	1:A:35:LEU:N	0.44	2.26	1	1
1:A:28:GLN:HE22	1:A:100:VAL:C	0.44	2.21	5	1
1:A:23:GLN:O	1:A:24:ASP:CG	0.44	2.61	8	7
1:A:95:ALA:C	1:A:97:ARG:N	0.44	2.75	1	1
1:A:28:GLN:CD	1:A:100:VAL:O	0.44	2.61	5	1
1:A:28:GLN:NE2	1:A:99:THR:CG2	0.43	2.81	5	1
1:A:25:LEU:N	1:A:25:LEU:CD1	0.43	2.80	2	1
1:A:107:TYR:CD1	1:A:107:TYR:N	0.43	2.87	1	2
1:A:80:PHE:CE1	1:A:84:VAL:HG21	0.43	2.48	4	3
1:A:95:ALA:O	1:A:96:LYS:C	0.42	2.62	1	4
1:A:15:THR:OG1	1:A:81:LEU:HD13	0.42	2.15	3	1
1:A:19:THR:O	1:A:22:ASP:OD2	0.42	2.37	9	1
1:A:12:LYS:HZ1	1:A:32:ILE:HD11	0.42	1.74	3	1
1:A:40:GLU:CD	1:A:40:GLU:C	0.42	2.88	6	2
1:A:11:VAL:CG1	1:A:12:LYS:N	0.42	2.82	9	2
1:A:31:ALA:O	1:A:35:LEU:HD13	0.42	2.15	2	1
1:A:37:GLU:O	1:A:41:ALA:CB	0.42	2.67	6	4
1:A:19:THR:O	1:A:20:THR:C	0.41	2.64	10	4
1:A:30:MET:O	1:A:31:ALA:C	0.41	2.64	4	1
1:A:84:VAL:O	1:A:88:SER:N	0.41	2.53	9	1
1:A:80:PHE:O	1:A:84:VAL:CG2	0.40	2.63	4	1
1:A:103:LEU:C	1:A:103:LEU:CD1	0.40	2.94	2	1
1:A:98:LYS:O	1:A:99:THR:OG1	0.40	2.37	6	2

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/121 (58%)	64±1 (91±1%)	3±1 (4±1%)	4±1 (5±1%)	3	23
All	All	700/1210 (58%)	638 (91%)	26 (4%)	36 (5%)	3	23

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	20	THR	10
1	A	21	LYS	10
1	A	24	ASP	8
1	A	96	LYS	5
1	A	22	ASP	3

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/105 (59%)	58±2 (94±2%)	4±2 (6±2%)	21	70
All	All	620/1050 (59%)	585 (94%)	35 (6%)	21	70

All 9 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	23	GLN	10
1	A	96	LYS	9
1	A	76	VAL	4
1	A	98	LYS	4
1	A	103	LEU	3
1	A	35	LEU	2
1	A	28	GLN	1
1	A	19	THR	1
1	A	85	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1446
Number of shifts mapped to atoms	1446
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	117	-0.38 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	0.26 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	111	0.06 ± 0.12	None needed (< 0.5 ppm)
^{15}N	111	0.22 ± 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 862 atoms were assigned a chemical shift out of a possible 976. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	343/350 (98%)	137/140 (98%)	139/140 (99%)	67/70 (96%)
Sidechain	495/559 (89%)	338/365 (93%)	154/174 (89%)	3/20 (15%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	24/67 (36%)	24/33 (73%)	0/32 (0%)	0/2 (0%)
Overall	862/976 (88%)	499/538 (93%)	293/346 (85%)	70/92 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1446 atoms were assigned a chemical shift out of a possible 1725. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	574/608 (94%)	235/247 (95%)	228/242 (94%)	111/119 (93%)
Sidechain	831/999 (83%)	567/654 (87%)	259/305 (85%)	5/40 (12%)
Aromatic	41/118 (35%)	41/58 (71%)	0/56 (0%)	0/4 (0%)
Overall	1446/1725 (84%)	843/959 (88%)	487/603 (81%)	116/163 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

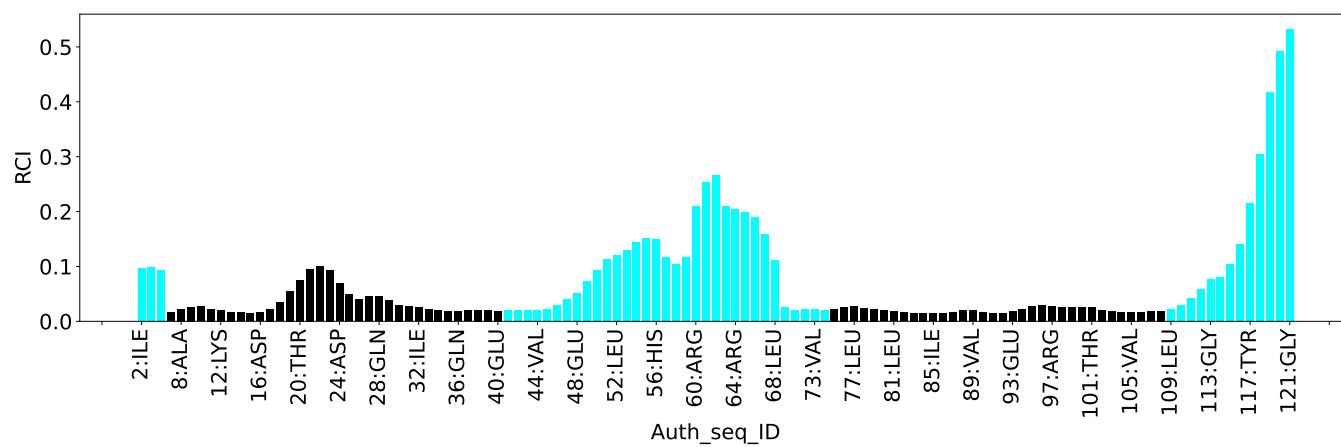
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	SER	HB2	2.59	2.61 – 5.13	-5.1

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3334
Intra-residue ($ i-j =0$)	779
Sequential ($ i-j =1$)	850
Medium range ($ i-j >1$ and $ i-j <5$)	1150
Long range ($ i-j \geq 5$)	437
Inter-chain	0
Hydrogen bond restraints	118
Disulfide bond restraints	0
Total dihedral-angle restraints	190
Number of unmapped restraints	0
Number of restraints per residue	29.1
Number of long range restraints per residue ¹	3.6

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)	168.7	0.2
0.2-0.5 (Medium)	123.0	0.49
>0.5 (Large)	5.1	3.64

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.5	7.04
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

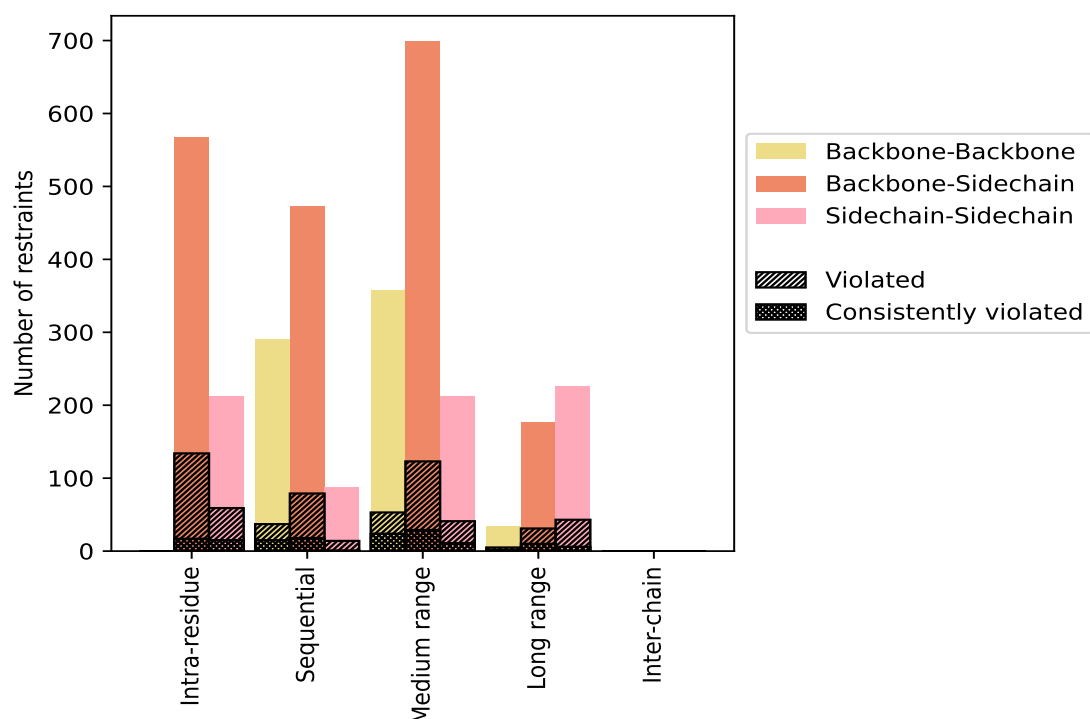
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	779	23.4	193	24.8	5.8	32	4.1	1.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	567	17.0	134	23.6	4.0	17	3.0	0.5
Sidechain-Sidechain	212	6.4	59	27.8	1.8	15	7.1	0.4
Sequential ($i-j =1$)	850	25.5	130	15.3	3.9	34	4.0	1.0
Backbone-Backbone	290	8.7	37	12.8	1.1	15	5.2	0.4
Backbone-Sidechain	473	14.2	79	16.7	2.4	18	3.8	0.5
Sidechain-Sidechain	87	2.6	14	16.1	0.4	1	1.1	0.0
Medium range ($i-j >1$ & $i-j <5$)	1150	34.5	203	17.7	6.1	63	5.5	1.9
Backbone-Backbone	357	10.7	53	14.8	1.6	24	6.7	0.7
Backbone-Sidechain	581	17.4	109	18.8	3.3	28	4.8	0.8
Sidechain-Sidechain	212	6.4	41	19.3	1.2	11	5.2	0.3
Long range ($i-j \geq 5$)	437	13.1	79	18.1	2.4	18	4.1	0.5
Backbone-Backbone	34	1.0	5	14.7	0.1	2	5.9	0.1
Backbone-Sidechain	177	5.3	31	17.5	0.9	10	5.6	0.3
Sidechain-Sidechain	226	6.8	43	19.0	1.3	6	2.7	0.2
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	118	3.5	14	11.9	0.4	1	0.8	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3334	100.0	619	18.6	18.6	148	4.4	4.4
Backbone-Backbone	681	20.4	95	14.0	2.8	41	6.0	1.2
Backbone-Sidechain	1916	57.5	367	19.2	11.0	74	3.9	2.2
Sidechain-Sidechain	737	22.1	157	21.3	4.7	33	4.5	1.0

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

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



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

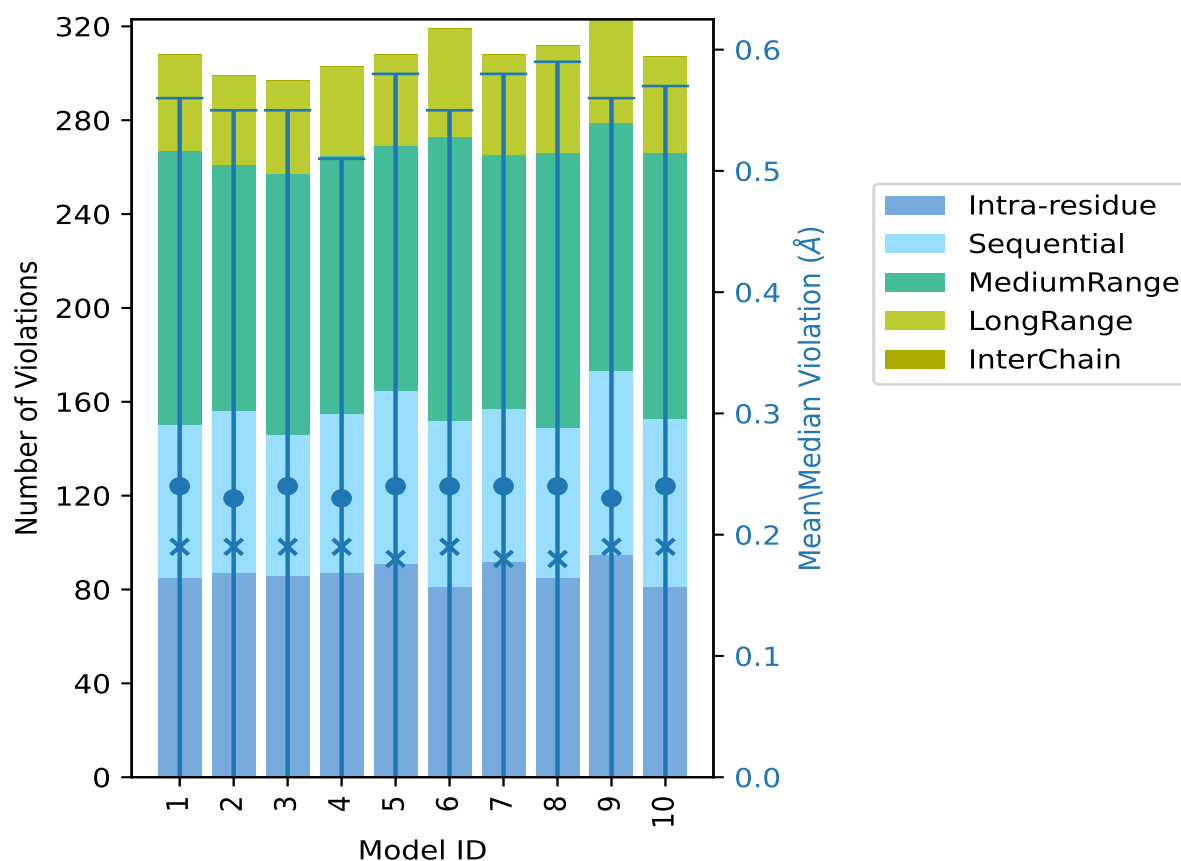
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	85	65	117	41	0	308	0.24	3.2	0.32	0.19
2	87	69	105	38	0	299	0.23	3.31	0.32	0.19
3	86	60	111	40	0	297	0.24	3.03	0.31	0.19
4	87	68	110	38	0	303	0.23	2.89	0.28	0.19
5	91	74	104	39	0	308	0.24	3.58	0.34	0.18
6	81	71	121	46	0	319	0.24	3.16	0.31	0.19
7	92	65	108	43	0	308	0.24	3.47	0.34	0.18
8	85	64	117	46	0	312	0.24	3.64	0.35	0.18
9	95	78	106	44	0	323	0.23	3.52	0.33	0.19
10	81	72	113	41	0	307	0.24	3.34	0.33	0.19

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2611(IR:586, SQ:720, MR:947, LR:358, 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	%
57	30	55	19	0	161	1	10.0
27	17	23	13	0	80	2	20.0
15	14	17	2	0	48	3	30.0

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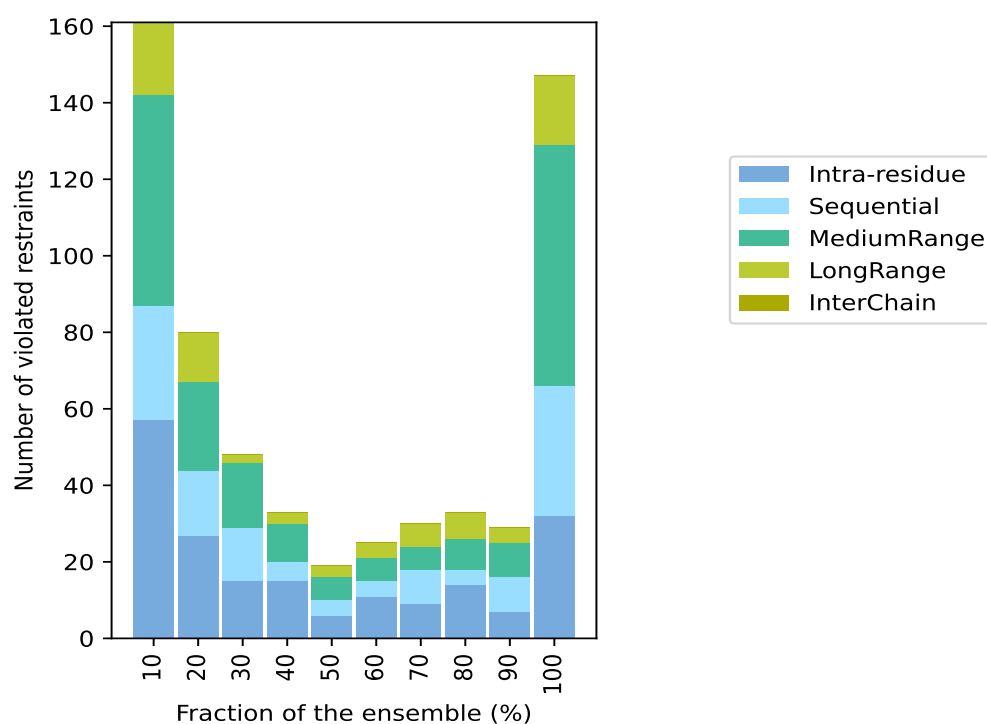
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
15	5	10	3	0	33	4	40.0
6	4	6	3	0	19	5	50.0
11	4	6	4	0	25	6	60.0
9	9	6	6	0	30	7	70.0
14	4	8	7	0	33	8	80.0
7	9	9	4	0	29	9	90.0
32	34	63	18	0	147	10	100.0

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 ⓘ

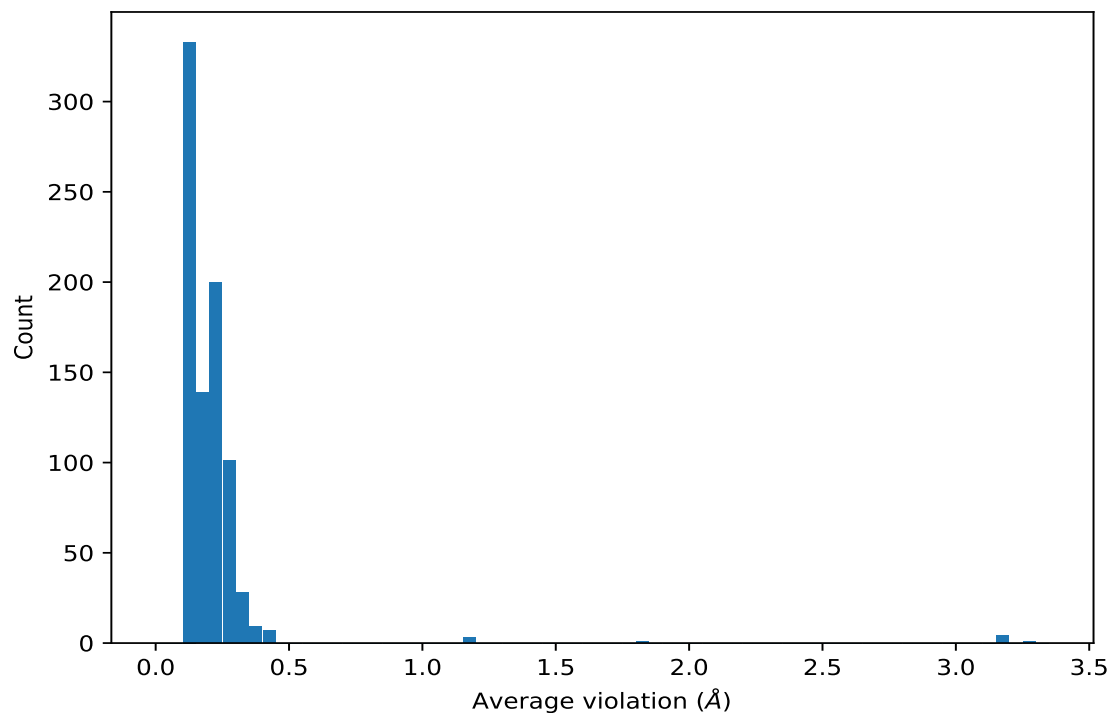


9.4 Most violated distance restraints in the ensemble ⓘ

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)
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	10	3.3	0.26	3.32
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	10	3.19	0.17	3.15
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	10	3.17	0.18	3.18
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	10	3.17	0.18	3.18
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	10	3.17	0.18	3.18
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	10	1.81	0.14	1.81
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	10	0.4	0.04	0.4
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	10	0.39	0.02	0.39
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	10	0.38	0.02	0.38
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	10	0.38	0.03	0.36
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	10	0.38	0.03	0.36
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	10	0.37	0.04	0.39
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	10	0.37	0.04	0.39
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	10	0.37	0.04	0.39
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	10	0.34	0.02	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	10	0.34	0.01	0.34
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	10	0.33	0.02	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	10	0.33	0.02	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	10	0.33	0.02	0.33
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	10	0.33	0.03	0.34
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	10	0.33	0.0	0.33
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	10	0.33	0.03	0.32
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	10	0.33	0.03	0.34
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	10	0.33	0.03	0.33
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	10	0.32	0.02	0.32
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	10	0.32	0.02	0.32
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	10	0.32	0.02	0.32
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	10	0.32	0.02	0.32
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	10	0.32	0.01	0.32
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	10	0.31	0.04	0.33
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	10	0.31	0.03	0.3
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	10	0.31	0.06	0.34
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	10	0.3	0.02	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	10	0.3	0.01	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	10	0.3	0.01	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	10	0.3	0.01	0.3
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	10	0.3	0.05	0.3
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	10	0.29	0.06	0.31
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	10	0.29	0.03	0.3
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	10	0.29	0.02	0.29
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	10	0.28	0.04	0.26
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	10	0.28	0.02	0.28
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	10	0.28	0.03	0.28
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	10	0.28	0.05	0.28
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	10	0.27	0.05	0.29
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	10	0.27	0.04	0.29
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	10	0.27	0.04	0.29
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	10	0.27	0.04	0.29
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	10	0.27	0.02	0.27
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	10	0.27	0.01	0.27
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	10	0.27	0.01	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	10	0.27	0.01	0.27
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	10	0.27	0.02	0.27
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	10	0.27	0.02	0.27
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	10	0.27	0.02	0.27
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	10	0.27	0.02	0.28
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	10	0.27	0.0	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	10	0.27	0.03	0.27
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	10	0.26	0.02	0.26
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	10	0.26	0.03	0.26
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	10	0.26	0.03	0.27
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	10	0.26	0.01	0.26
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	10	0.26	0.01	0.26
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	10	0.26	0.03	0.26
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	10	0.26	0.01	0.26
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	10	0.25	0.07	0.24
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	10	0.25	0.07	0.24
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	10	0.25	0.01	0.25
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	10	0.25	0.01	0.25
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	10	0.25	0.01	0.25
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	10	0.25	0.07	0.24
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	10	0.24	0.03	0.23
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	10	0.24	0.06	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	10	0.24	0.06	0.22
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	10	0.24	0.02	0.24
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	10	0.24	0.02	0.24
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	10	0.24	0.02	0.24
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	10	0.24	0.04	0.24
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	10	0.24	0.02	0.24
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	10	0.24	0.02	0.24
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	10	0.24	0.02	0.24
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	10	0.24	0.04	0.25
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	10	0.24	0.0	0.24
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	10	0.24	0.01	0.23
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	10	0.23	0.02	0.24
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	10	0.23	0.05	0.22
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	10	0.23	0.03	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	10	0.23	0.01	0.23
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	10	0.23	0.02	0.22
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	10	0.23	0.02	0.24
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	10	0.22	0.01	0.22
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	10	0.22	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	10	0.22	0.05	0.23
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	10	0.22	0.05	0.23
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	10	0.22	0.01	0.22
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	10	0.22	0.04	0.21
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	10	0.22	0.05	0.22
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	10	0.22	0.04	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	10	0.22	0.01	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	10	0.22	0.01	0.22
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	10	0.22	0.01	0.22
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	10	0.22	0.01	0.22
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	10	0.22	0.01	0.22
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	10	0.22	0.02	0.22
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	10	0.22	0.05	0.2
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	10	0.22	0.04	0.2
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	10	0.22	0.03	0.22
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	10	0.21	0.04	0.21
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	10	0.21	0.02	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	10	0.21	0.03	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	10	0.21	0.03	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	10	0.21	0.03	0.22
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	10	0.21	0.01	0.21
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	10	0.21	0.03	0.22
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	10	0.21	0.01	0.21
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	10	0.21	0.04	0.19
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	10	0.21	0.03	0.22
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	10	0.21	0.03	0.21
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	10	0.2	0.03	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	10	0.2	0.03	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	10	0.2	0.01	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	10	0.2	0.05	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	10	0.2	0.05	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	10	0.2	0.05	0.2
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	10	0.2	0.02	0.19
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	10	0.2	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	10	0.2	0.02	0.19
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	10	0.2	0.02	0.19
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	10	0.2	0.02	0.19
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	10	0.2	0.02	0.19
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	10	0.2	0.01	0.2
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	10	0.2	0.02	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	10	0.19	0.01	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	10	0.19	0.01	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	10	0.19	0.01	0.2
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	10	0.19	0.03	0.2
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	10	0.19	0.03	0.19
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	10	0.19	0.03	0.19
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	10	0.19	0.04	0.2
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	10	0.19	0.03	0.2
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	10	0.19	0.0	0.19
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	10	0.19	0.06	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	10	0.18	0.01	0.18
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	10	0.18	0.02	0.19
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	10	0.18	0.0	0.18
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	10	0.18	0.04	0.17
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	10	0.18	0.02	0.18
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	10	0.18	0.02	0.18
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	10	0.18	0.02	0.18
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	10	0.18	0.02	0.17
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	10	0.18	0.02	0.18
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	10	0.18	0.02	0.18
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	10	0.18	0.02	0.18
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	10	0.18	0.04	0.17
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	10	0.18	0.03	0.18
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	10	0.18	0.02	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	10	0.18	0.01	0.17
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	10	0.17	0.01	0.18
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	10	0.17	0.02	0.17
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	10	0.17	0.01	0.17
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	10	0.17	0.04	0.17
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	10	0.17	0.03	0.16
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	10	0.17	0.02	0.16
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	10	0.17	0.02	0.16
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	10	0.17	0.02	0.16
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	10	0.17	0.02	0.16
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	10	0.17	0.02	0.16
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	10	0.17	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	10	0.17	0.03	0.17
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	10	0.16	0.02	0.16
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	10	0.16	0.03	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	10	0.16	0.03	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	10	0.16	0.03	0.15
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	10	0.16	0.02	0.16
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	10	0.16	0.05	0.15
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	10	0.16	0.03	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	10	0.16	0.01	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	10	0.15	0.01	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	10	0.15	0.01	0.16
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	10	0.15	0.02	0.16
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	10	0.15	0.03	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	10	0.15	0.03	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	10	0.15	0.03	0.15
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	10	0.15	0.04	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	10	0.15	0.04	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	10	0.15	0.04	0.15
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	10	0.15	0.01	0.15
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	10	0.15	0.02	0.15
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	10	0.15	0.01	0.15
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	10	0.15	0.03	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	10	0.14	0.01	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	10	0.14	0.01	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	10	0.14	0.01	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	10	0.14	0.04	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	10	0.14	0.04	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	10	0.14	0.04	0.13
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	10	0.14	0.01	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	10	0.14	0.02	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	10	0.14	0.02	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	10	0.14	0.02	0.14
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	10	0.13	0.01	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	10	0.13	0.01	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	10	0.13	0.01	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	10	0.13	0.01	0.13
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	10	0.12	0.01	0.12
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	10	0.12	0.01	0.12
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	10	0.12	0.01	0.12
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	10	0.12	0.01	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	10	0.12	0.01	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	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)
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	10	0.12	0.01	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	10	0.12	0.01	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	10	0.12	0.01	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	10	0.12	0.01	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	10	0.12	0.01	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	10	0.12	0.01	0.12
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	10	0.11	0.01	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	10	0.11	0.01	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	10	0.11	0.01	0.11
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	9	0.34	0.07	0.36
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	9	0.29	0.01	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	9	0.29	0.01	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	9	0.29	0.01	0.29
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	9	0.28	0.01	0.28
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	9	0.24	0.2	0.14
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	9	0.23	0.01	0.23
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	9	0.2	0.01	0.2
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	9	0.2	0.01	0.2
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	9	0.2	0.01	0.2
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	9	0.2	0.03	0.19
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	9	0.2	0.05	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	9	0.2	0.05	0.21
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	9	0.2	0.03	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	9	0.2	0.03	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	9	0.2	0.03	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	9	0.2	0.03	0.2
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	9	0.19	0.02	0.18
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	9	0.18	0.03	0.18
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	9	0.18	0.04	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	9	0.18	0.03	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	9	0.18	0.03	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	9	0.18	0.03	0.18
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	9	0.18	0.07	0.14
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	9	0.17	0.05	0.16
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	9	0.17	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	9	0.17	0.03	0.17
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	9	0.16	0.03	0.16
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	9	0.16	0.06	0.14
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	9	0.16	0.06	0.14
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	9	0.16	0.0	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	9	0.16	0.0	0.16
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	9	0.15	0.02	0.15
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	9	0.15	0.04	0.13
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	9	0.14	0.03	0.16
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	9	0.14	0.02	0.14
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	9	0.14	0.02	0.14
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	9	0.14	0.02	0.14
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	9	0.13	0.03	0.12
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	9	0.13	0.02	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	9	0.13	0.0	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	9	0.13	0.0	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	9	0.13	0.0	0.13
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	9	0.12	0.01	0.12
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	9	0.12	0.01	0.12
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	9	0.12	0.01	0.12
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	8	1.16	0.4	1.27
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	8	1.16	0.4	1.27
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	8	1.16	0.4	1.27
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	8	0.35	0.02	0.35
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	8	0.28	0.01	0.28
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	8	0.24	0.03	0.24
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	8	0.24	0.03	0.24
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	8	0.23	0.0	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	8	0.22	0.03	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	8	0.22	0.03	0.22
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	8	0.22	0.03	0.22
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	8	0.22	0.04	0.22
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	8	0.21	0.01	0.2
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	8	0.2	0.04	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	8	0.2	0.04	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	8	0.2	0.04	0.22
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	8	0.2	0.02	0.2
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	8	0.19	0.08	0.18
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	8	0.18	0.04	0.19
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	8	0.18	0.09	0.14
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	8	0.17	0.04	0.18
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	8	0.17	0.04	0.18
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	8	0.17	0.04	0.18
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	8	0.16	0.01	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	8	0.16	0.01	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	8	0.16	0.01	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	8	0.16	0.02	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	8	0.16	0.02	0.16
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	8	0.16	0.07	0.15
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	8	0.16	0.03	0.17
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	8	0.16	0.04	0.16
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	8	0.15	0.01	0.16
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	8	0.15	0.01	0.16
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	8	0.15	0.01	0.16
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	8	0.15	0.02	0.15
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	8	0.15	0.02	0.15
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	8	0.15	0.02	0.15
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	8	0.15	0.03	0.14
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	8	0.15	0.03	0.15
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	8	0.15	0.02	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	8	0.15	0.01	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	8	0.15	0.01	0.15
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	8	0.15	0.02	0.16
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	8	0.14	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	8	0.14	0.02	0.14
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	8	0.14	0.01	0.14
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	8	0.13	0.01	0.12
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	8	0.13	0.02	0.13
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	8	0.12	0.01	0.12
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	8	0.12	0.01	0.12
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	8	0.12	0.01	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	8	0.12	0.0	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	8	0.12	0.0	0.12
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	8	0.12	0.0	0.12
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	8	0.1	0.0	0.1
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	7	0.32	0.08	0.27
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	7	0.31	0.01	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	7	0.31	0.0	0.31
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	7	0.3	0.01	0.3
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	7	0.3	0.01	0.3
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	7	0.3	0.01	0.3
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	7	0.27	0.04	0.25
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	7	0.27	0.04	0.25
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	7	0.22	0.03	0.21
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	7	0.22	0.03	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	7	0.22	0.03	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	7	0.22	0.03	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	7	0.22	0.03	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	7	0.22	0.03	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	7	0.22	0.03	0.23
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	7	0.21	0.01	0.21
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	7	0.21	0.01	0.21
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	7	0.18	0.03	0.17
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	7	0.18	0.03	0.17
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	7	0.18	0.02	0.18
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	7	0.17	0.04	0.19
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	7	0.17	0.04	0.19
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	7	0.17	0.04	0.19
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	7	0.17	0.04	0.16
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	7	0.17	0.03	0.17
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	7	0.17	0.03	0.17
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	7	0.17	0.03	0.17
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	7	0.14	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	7	0.14	0.04	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	7	0.14	0.04	0.13
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	7	0.14	0.01	0.14
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	7	0.14	0.01	0.14
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	7	0.14	0.03	0.14
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	7	0.14	0.04	0.12
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	7	0.14	0.04	0.12
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	7	0.13	0.0	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	7	0.13	0.0	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	7	0.13	0.0	0.13
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	7	0.13	0.01	0.14
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	7	0.13	0.01	0.13
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	7	0.13	0.02	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	7	0.13	0.02	0.12
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	7	0.13	0.02	0.13
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	7	0.13	0.02	0.13
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	7	0.13	0.01	0.13
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	7	0.13	0.01	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	7	0.13	0.01	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	7	0.13	0.01	0.12
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	7	0.13	0.02	0.12
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	7	0.12	0.01	0.12
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	7	0.11	0.01	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	7	0.11	0.01	0.11
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	7	0.11	0.01	0.11
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	6	0.38	0.03	0.36
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	6	0.31	0.01	0.3
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	6	0.27	0.01	0.26
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	6	0.26	0.01	0.27
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	6	0.26	0.01	0.27
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	6	0.26	0.01	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	6	0.26	0.03	0.27
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	6	0.26	0.03	0.27
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	6	0.26	0.03	0.27
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	6	0.24	0.01	0.24
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	6	0.24	0.04	0.24
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	6	0.2	0.18	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	6	0.2	0.18	0.12
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	6	0.2	0.01	0.2
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	6	0.2	0.01	0.2
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	6	0.2	0.01	0.2
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	6	0.19	0.05	0.2
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	6	0.19	0.03	0.17
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	6	0.18	0.06	0.16
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	6	0.16	0.02	0.16
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	6	0.16	0.05	0.14
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	6	0.15	0.01	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	6	0.15	0.01	0.15
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	6	0.15	0.03	0.14
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	6	0.15	0.03	0.14
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	6	0.14	0.02	0.14
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	6	0.14	0.02	0.14
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	6	0.14	0.02	0.14
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	6	0.14	0.05	0.12
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	6	0.13	0.03	0.12
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	6	0.13	0.03	0.12
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	6	0.13	0.03	0.12
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	6	0.13	0.01	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	6	0.13	0.01	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	6	0.13	0.01	0.13
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	6	0.13	0.03	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	6	0.13	0.03	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	6	0.13	0.03	0.11
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	6	0.13	0.03	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	6	0.12	0.02	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	6	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	6	0.12	0.02	0.11
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	6	0.12	0.02	0.11
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	6	0.12	0.02	0.11
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	6	0.12	0.02	0.11
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	6	0.11	0.0	0.11
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	5	0.41	0.03	0.41
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	5	0.41	0.03	0.41
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	5	0.41	0.03	0.41
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	5	0.3	0.1	0.33
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	5	0.3	0.1	0.33
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	5	0.3	0.1	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	5	0.3	0.1	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	5	0.3	0.1	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	5	0.3	0.1	0.33
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	5	0.27	0.11	0.24
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	5	0.25	0.11	0.23
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	5	0.25	0.11	0.23
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	5	0.25	0.11	0.23
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	5	0.23	0.03	0.22
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	5	0.23	0.03	0.22
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	5	0.23	0.03	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	5	0.2	0.02	0.21
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	5	0.2	0.02	0.21
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	5	0.2	0.02	0.21
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	5	0.19	0.1	0.16
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	5	0.19	0.06	0.16
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	5	0.19	0.06	0.16
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	5	0.19	0.06	0.16
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	5	0.15	0.02	0.16
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	5	0.15	0.02	0.16
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	5	0.15	0.02	0.16
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	5	0.15	0.03	0.15
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	5	0.15	0.03	0.15
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	5	0.15	0.03	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	5	0.15	0.03	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	5	0.15	0.03	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	5	0.15	0.03	0.15
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	5	0.14	0.01	0.14
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	5	0.14	0.02	0.14
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	5	0.13	0.02	0.13
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	5	0.13	0.02	0.12
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	5	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	5	0.13	0.02	0.12
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	5	0.13	0.01	0.12
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	5	0.12	0.01	0.12
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	5	0.12	0.02	0.12
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	5	0.12	0.01	0.12
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	5	0.11	0.0	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	5	0.11	0.0	0.11
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	5	0.11	0.01	0.11
(1,2940)	1:107:A:TYR:HD2	1:108:A:ALA:H	4	0.35	0.01	0.36
(1,995)	1:103:A:LEU:HD11	1:105:A:VAL:HB	4	0.3	0.07	0.26
(1,995)	1:103:A:LEU:HD12	1:105:A:VAL:HB	4	0.3	0.07	0.26
(1,995)	1:103:A:LEU:HD13	1:105:A:VAL:HB	4	0.3	0.07	0.26
(1,707)	1:74:A:ARG:HD2	1:74:A:ARG:HB3	4	0.3	0.01	0.3
(1,1968)	1:48:A:GLU:HG3	1:48:A:GLU:H	4	0.3	0.02	0.3
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB1	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB2	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB3	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB1	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB2	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB3	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB1	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB2	4	0.28	0.08	0.31
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB3	4	0.28	0.08	0.31
(1,1086)	1:110:A:LYS:HE2	1:110:A:LYS:HB2	4	0.26	0.0	0.26
(1,1086)	1:110:A:LYS:HE3	1:110:A:LYS:HB2	4	0.26	0.0	0.26
(1,2163)	1:68:A:LEU:HG	1:68:A:LEU:H	4	0.23	0.17	0.15
(1,2028)	1:51:A:ASN:H	1:53:A:LEU:H	4	0.22	0.12	0.17
(1,2095)	1:58:A:VAL:HG11	1:58:A:VAL:H	4	0.22	0.02	0.22
(1,2095)	1:58:A:VAL:HG12	1:58:A:VAL:H	4	0.22	0.02	0.22
(1,2095)	1:58:A:VAL:HG13	1:58:A:VAL:H	4	0.22	0.02	0.22
(1,2000)	1:50:A:THR:HB	1:51:A:ASN:H	4	0.2	0.08	0.2
(1,991)	1:103:A:LEU:HD11	1:103:A:LEU:HA	4	0.2	0.11	0.15
(1,991)	1:103:A:LEU:HD12	1:103:A:LEU:HA	4	0.2	0.11	0.15
(1,991)	1:103:A:LEU:HD13	1:103:A:LEU:HA	4	0.2	0.11	0.15
(1,2732)	1:96:A:LYS:HD3	1:96:A:LYS:H	4	0.2	0.02	0.19
(1,950)	1:96:A:LYS:HD3	1:96:A:LYS:HB2	4	0.18	0.03	0.2
(1,2141)	1:65:A:ILE:HG12	1:65:A:ILE:H	4	0.18	0.06	0.2
(1,962)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	4	0.18	0.02	0.17
(1,1133)	1:116:A:LEU:HA	1:116:A:LEU:HG	4	0.17	0.04	0.16
(1,2090)	1:57:A:LEU:HG	1:58:A:VAL:H	4	0.17	0.04	0.16
(1,2712)	1:94:A:HIS:H	1:96:A:LYS:HG3	4	0.17	0.01	0.16
(1,1611)	1:30:A:MET:HG2	1:30:A:MET:H	4	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3064)	1:114:A:ARG:H	1:115:A:THR:HA	4	0.15	0.03	0.15
(1,2703)	1:93:A:GLU:HA	1:98:A:LYS:H	4	0.15	0.04	0.14
(1,2071)	1:55:A:LEU:H	1:57:A:LEU:H	4	0.14	0.02	0.14
(1,868)	1:87:A:ASP:HB3	1:104:A:ASP:HB3	4	0.14	0.02	0.15
(1,1216)	1:9:A:ARG:H	1:11:A:VAL:H	4	0.14	0.01	0.14
(1,3036)	1:112:A:GLN:HB2	1:112:A:GLN:HE21	4	0.14	0.02	0.12
(1,2950)	1:107:A:TYR:H	1:110:A:LYS:HB2	4	0.13	0.03	0.12
(1,3130)	1:15:A:THR:HA	1:18:A:PHE:HZ	4	0.13	0.02	0.13
(1,2804)	1:101:A:THR:HA	1:103:A:LEU:H	4	0.12	0.02	0.12
(1,1056)	1:108:A:ALA:HB1	1:111:A:ARG:HB2	4	0.12	0.0	0.12
(1,1056)	1:108:A:ALA:HB2	1:111:A:ARG:HB2	4	0.12	0.0	0.12
(1,1056)	1:108:A:ALA:HB3	1:111:A:ARG:HB2	4	0.12	0.0	0.12
(1,2136)	1:64:A:ARG:HA	1:65:A:ILE:H	4	0.12	0.02	0.12
(1,2484)	1:84:A:VAL:HA	1:112:A:GLN:HE21	4	0.12	0.0	0.12
(1,165)	1:21:A:LYS:HD2	1:21:A:LYS:HA	4	0.11	0.01	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG11	4	0.11	0.0	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG12	4	0.11	0.0	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG13	4	0.11	0.0	0.11
(1,2444)	1:83:A:SER:HB3	1:84:A:VAL:H	3	0.44	0.0	0.44
(1,3086)	1:116:A:LEU:HA	1:117:A:TYR:H	3	0.33	0.05	0.36
(1,2249)	1:74:A:ARG:HB2	1:76:A:VAL:H	3	0.31	0.02	0.31
(1,1344)	1:15:A:THR:H	1:17:A:GLU:HG2	3	0.3	0.0	0.3
(1,2004)	1:51:A:ASN:HB3	1:51:A:ASN:H	3	0.3	0.11	0.29
(1,2139)	1:64:A:ARG:H	1:65:A:ILE:H	3	0.28	0.05	0.31
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB1	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB2	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB3	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB1	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB2	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB3	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB1	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB2	3	0.24	0.03	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB3	3	0.24	0.03	0.23
(1,624)	1:65:A:ILE:HA	1:65:A:ILE:HG12	3	0.23	0.06	0.2
(1,3077)	1:115:A:THR:HB	1:116:A:LEU:H	3	0.23	0.1	0.21
(1,2437)	1:83:A:SER:HB3	1:83:A:SER:H	3	0.22	0.0	0.22
(1,2041)	1:52:A:LEU:H	1:53:A:LEU:HA	3	0.2	0.0	0.2
(1,2749)	1:97:A:ARG:HG2	1:97:A:ARG:HE	3	0.2	0.07	0.15
(1,2026)	1:51:A:ASN:HB3	1:53:A:LEU:H	3	0.2	0.09	0.14
(1,398)	1:40:A:GLU:HG3	1:41:A:ALA:HA	3	0.19	0.0	0.19
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD11	3	0.18	0.05	0.19
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD12	3	0.18	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD13	3	0.18	0.05	0.19
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD2	3	0.18	0.06	0.22
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD3	3	0.18	0.06	0.22
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD2	3	0.17	0.04	0.2
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD3	3	0.17	0.04	0.2
(1,2542)	1:87:A:ASP:HB3	1:88:A:SER:H	3	0.17	0.02	0.18
(1,71)	1:11:A:VAL:HG11	1:35:A:LEU:HG	3	0.17	0.05	0.18
(1,71)	1:11:A:VAL:HG12	1:35:A:LEU:HG	3	0.17	0.05	0.18
(1,71)	1:11:A:VAL:HG13	1:35:A:LEU:HG	3	0.17	0.05	0.18
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD11	3	0.17	0.03	0.16
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD12	3	0.17	0.03	0.16
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD13	3	0.17	0.03	0.16
(1,2853)	1:103:A:LEU:HG	1:105:A:VAL:H	3	0.17	0.01	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG21	3	0.15	0.03	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG22	3	0.15	0.03	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG23	3	0.15	0.03	0.16
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD11	3	0.15	0.0	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD12	3	0.15	0.0	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD13	3	0.15	0.0	0.15
(1,1116)	1:114:A:ARG:HB3	1:114:A:ARG:HD3	3	0.15	0.02	0.16
(1,1152)	1:117:A:TYR:HB2	1:119:A:PHE:HB3	3	0.15	0.02	0.15
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG21	3	0.15	0.03	0.16
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG22	3	0.15	0.03	0.16
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG23	3	0.15	0.03	0.16
(1,1530)	1:26:A:ARG:HD2	1:27:A:TRP:H	3	0.14	0.04	0.12
(1,2156)	1:66:A:SER:HB2	1:68:A:LEU:H	3	0.14	0.02	0.13
(1,2765)	1:98:A:LYS:HG3	1:98:A:LYS:H	3	0.14	0.02	0.15
(1,3095)	1:117:A:TYR:HB3	1:117:A:TYR:H	3	0.14	0.03	0.12
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	3	0.14	0.02	0.15
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	3	0.14	0.02	0.15
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG2	3	0.14	0.0	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG3	3	0.14	0.0	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG2	3	0.14	0.0	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG3	3	0.14	0.0	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG2	3	0.14	0.0	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG3	3	0.14	0.0	0.14
(1,968)	1:98:A:LYS:HA	1:98:A:LYS:HG2	3	0.14	0.0	0.14
(1,637)	1:68:A:LEU:HG	1:68:A:LEU:HA	3	0.14	0.01	0.13
(1,1218)	1:9:A:ARG:HB2	1:11:A:VAL:H	3	0.13	0.01	0.12
(1,1219)	1:9:A:ARG:H	1:12:A:LYS:H	3	0.12	0.02	0.13
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD11	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD12	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD13	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD11	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD12	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD13	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD11	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD12	3	0.12	0.01	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD13	3	0.12	0.01	0.12
(1,3099)	1:117:A:TYR:HB3	1:118:A:GLY:H	3	0.12	0.01	0.12
(1,932)	1:93:A:GLU:HA	1:96:A:LYS:HA	3	0.12	0.0	0.12
(1,1372)	1:17:A:GLU:HG2	1:17:A:GLU:H	3	0.12	0.01	0.11
(1,2445)	1:83:A:SER:HB2	1:84:A:VAL:H	3	0.12	0.0	0.12
(1,2939)	1:107:A:TYR:HB3	1:108:A:ALA:H	3	0.11	0.01	0.12
(1,1932)	1:46:A:LEU:HB2	1:47:A:LEU:H	3	0.11	0.0	0.11
(1,2702)	1:93:A:GLU:HA	1:97:A:ARG:H	3	0.11	0.0	0.11
(1,1246)	1:11:A:VAL:HG21	1:11:A:VAL:H	3	0.1	0.0	0.1
(1,1246)	1:11:A:VAL:HG22	1:11:A:VAL:H	3	0.1	0.0	0.1
(1,1246)	1:11:A:VAL:HG23	1:11:A:VAL:H	3	0.1	0.0	0.1
(1,1707)	1:34:A:ALA:H	1:36:A:GLN:H	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB2	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB3	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB2	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB3	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB2	3	0.1	0.0	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB3	3	0.1	0.0	0.1
(1,2422)	1:82:A:GLU:HB2	1:83:A:SER:H	3	0.1	0.0	0.1
(1,2172)	1:69:A:ILE:HG13	1:69:A:ILE:H	2	0.42	0.01	0.42
(1,1343)	1:15:A:THR:HB	1:17:A:GLU:H	2	0.4	0.0	0.4
(1,1683)	1:33:A:MET:HB2	1:34:A:ALA:H	2	0.38	0.1	0.38
(1,1764)	1:37:A:GLU:HG2	1:37:A:GLU:H	2	0.32	0.02	0.32
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG11	2	0.29	0.01	0.29
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG12	2	0.29	0.01	0.29
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG13	2	0.29	0.01	0.29
(1,2007)	1:51:A:ASN:HB3	1:51:A:ASN:HD22	2	0.29	0.1	0.29
(1,3047)	1:112:A:GLN:HB3	1:113:A:GLY:H	2	0.28	0.06	0.28
(1,163)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	2	0.26	0.0	0.26
(1,163)	1:21:A:LYS:HE3	1:21:A:LYS:HB3	2	0.26	0.0	0.26
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB1	2	0.26	0.03	0.26
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB2	2	0.26	0.03	0.26
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB3	2	0.26	0.03	0.26
(1,890)	1:89:A:VAL:HG21	1:100:A:VAL:HA	2	0.26	0.03	0.26
(1,890)	1:89:A:VAL:HG22	1:100:A:VAL:HA	2	0.26	0.03	0.26
(1,890)	1:89:A:VAL:HG23	1:100:A:VAL:HA	2	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD11	2	0.25	0.1	0.25
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD12	2	0.25	0.1	0.25
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD13	2	0.25	0.1	0.25
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD11	2	0.24	0.07	0.24
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD12	2	0.24	0.07	0.24
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD13	2	0.24	0.07	0.24
(1,2160)	1:68:A:LEU:HB3	1:68:A:LEU:H	2	0.24	0.12	0.24
(1,186)	1:23:A:GLN:HG2	1:23:A:GLN:HA	2	0.23	0.01	0.23
(1,2134)	1:64:A:ARG:HB2	1:64:A:ARG:H	2	0.23	0.06	0.23
(1,313)	1:31:A:ALA:HA	1:33:A:MET:HB2	2	0.22	0.01	0.22
(1,1578)	1:28:A:GLN:HG2	1:28:A:GLN:H	2	0.22	0.01	0.22
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG21	2	0.22	0.02	0.22
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG22	2	0.22	0.02	0.22
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG23	2	0.22	0.02	0.22
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD11	2	0.22	0.03	0.22
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD12	2	0.22	0.03	0.22
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD13	2	0.22	0.03	0.22
(1,2757)	1:97:A:ARG:HB3	1:98:A:LYS:H	2	0.22	0.04	0.22
(1,1477)	1:23:A:GLN:HB2	1:24:A:ASP:H	2	0.21	0.05	0.21
(1,1585)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	2	0.21	0.02	0.21
(1,3010)	1:110:A:LYS:HB2	1:116:A:LEU:H	2	0.2	0.03	0.2
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD11	2	0.2	0.01	0.2
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD12	2	0.2	0.01	0.2
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD13	2	0.2	0.01	0.2
(1,3017)	1:111:A:ARG:H	1:112:A:GLN:HB3	2	0.2	0.06	0.2
(1,631)	1:65:A:ILE:HG21	1:68:A:LEU:HA	2	0.2	0.06	0.2
(1,631)	1:65:A:ILE:HG22	1:68:A:LEU:HA	2	0.2	0.06	0.2
(1,631)	1:65:A:ILE:HG23	1:68:A:LEU:HA	2	0.2	0.06	0.2
(1,1110)	1:113:A:GLY:HA2	1:114:A:ARG:HG3	2	0.2	0.06	0.2
(1,1304)	1:13:A:GLU:H	1:15:A:THR:HB	2	0.19	0.0	0.19
(1,2138)	1:64:A:ARG:HB3	1:65:A:ILE:H	2	0.19	0.03	0.19
(1,70)	1:11:A:VAL:HB	1:35:A:LEU:HA	2	0.18	0.02	0.18
(1,282)	1:28:A:GLN:HG3	1:99:A:THR:HA	2	0.18	0.05	0.18
(1,546)	1:53:A:LEU:HD21	1:57:A:LEU:HB2	2	0.18	0.08	0.18
(1,546)	1:53:A:LEU:HD22	1:57:A:LEU:HB2	2	0.18	0.08	0.18
(1,546)	1:53:A:LEU:HD23	1:57:A:LEU:HB2	2	0.18	0.08	0.18
(1,1250)	1:11:A:VAL:HB	1:12:A:LYS:H	2	0.18	0.0	0.18
(1,2173)	1:69:A:ILE:HG12	1:69:A:ILE:H	2	0.18	0.01	0.18
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG21	2	0.17	0.04	0.17
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG22	2	0.17	0.04	0.17
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG23	2	0.17	0.04	0.17
(1,2080)	1:56:A:HIS:HA	1:58:A:VAL:H	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2131)	1:63:A:LYS:H	1:64:A:ARG:HG3	2	0.16	0.04	0.16
(1,1441)	1:21:A:LYS:HB2	1:24:A:ASP:H	2	0.16	0.02	0.16
(1,2059)	1:54:A:ALA:HA	1:56:A:HIS:H	2	0.16	0.04	0.16
(1,2143)	1:65:A:ILE:HB	1:65:A:ILE:H	2	0.15	0.02	0.15
(1,2813)	1:101:A:THR:H	1:104:A:ASP:HB3	2	0.15	0.01	0.15
(2,26)	1:29:A:SER:O	1:33:A:MET:N	2	0.15	0.01	0.15
(1,2011)	1:51:A:ASN:HA	1:51:A:ASN:HD21	2	0.15	0.03	0.15
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD21	2	0.15	0.02	0.15
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD22	2	0.15	0.02	0.15
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD23	2	0.15	0.02	0.15
(1,964)	1:98:A:LYS:HD2	1:98:A:LYS:HB2	2	0.15	0.02	0.15
(1,3070)	1:114:A:ARG:HB2	1:115:A:THR:H	2	0.14	0.03	0.14
(1,803)	1:81:A:LEU:HA	1:84:A:VAL:HB	2	0.14	0.01	0.14
(1,806)	1:81:A:LEU:HA	1:84:A:VAL:HB	2	0.14	0.01	0.14
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD1	2	0.14	0.02	0.14
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD2	2	0.14	0.02	0.14
(1,40)	1:9:A:ARG:HD3	1:9:A:ARG:HB2	2	0.14	0.04	0.14
(1,2038)	1:52:A:LEU:HG	1:52:A:LEU:H	2	0.14	0.01	0.14
(1,2084)	1:57:A:LEU:HG	1:57:A:LEU:H	2	0.14	0.02	0.14
(1,2386)	1:80:A:PHE:HD1	1:112:A:GLN:HE22	2	0.14	0.01	0.14
(1,2386)	1:80:A:PHE:HD2	1:112:A:GLN:HE22	2	0.14	0.01	0.14
(1,1)	1:2:A:ILE:HG13	1:2:A:ILE:HA	2	0.13	0.0	0.13
(1,172)	1:21:A:LYS:HD2	1:85:A:ILE:HG12	2	0.13	0.02	0.13
(1,2273)	1:76:A:VAL:HB	1:77:A:LEU:H	2	0.13	0.03	0.13
(2,29)	1:31:A:ALA:O	1:35:A:LEU:H	2	0.13	0.02	0.13
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD2	2	0.12	0.01	0.12
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD3	2	0.12	0.01	0.12
(1,1081)	1:110:A:LYS:HA	1:110:A:LYS:HG3	2	0.12	0.01	0.12
(1,2075)	1:56:A:HIS:H	1:57:A:LEU:H	2	0.12	0.02	0.12
(1,3169)	1:41:A:ALA:HB1	1:80:A:PHE:HZ	2	0.12	0.02	0.12
(1,3169)	1:41:A:ALA:HB2	1:80:A:PHE:HZ	2	0.12	0.02	0.12
(1,3169)	1:41:A:ALA:HB3	1:80:A:PHE:HZ	2	0.12	0.02	0.12
(1,112)	1:14:A:VAL:HG21	1:17:A:GLU:HB2	2	0.12	0.01	0.12
(1,112)	1:14:A:VAL:HG22	1:17:A:GLU:HB2	2	0.12	0.01	0.12
(1,112)	1:14:A:VAL:HG23	1:17:A:GLU:HB2	2	0.12	0.01	0.12
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD11	2	0.12	0.01	0.12
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD12	2	0.12	0.01	0.12
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD13	2	0.12	0.01	0.12
(1,1788)	1:38:A:ALA:HA	1:41:A:ALA:H	2	0.12	0.01	0.12
(1,2152)	1:65:A:ILE:H	1:66:A:SER:HA	2	0.12	0.01	0.12
(1,3166)	1:38:A:ALA:HA	1:80:A:PHE:HZ	2	0.12	0.01	0.12
(1,2042)	1:52:A:LEU:HB2	1:54:A:ALA:H	2	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,95)	1:86:A:ARG:O	1:90:A:THR:H	2	0.12	0.0	0.12
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD21	2	0.11	0.01	0.11
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD22	2	0.11	0.01	0.11
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD23	2	0.11	0.01	0.11
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD21	2	0.11	0.01	0.11
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD22	2	0.11	0.01	0.11
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD23	2	0.11	0.01	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,355)	1:34:A:ALA:HB1	1:105:A:VAL:HB	2	0.11	0.01	0.11
(1,355)	1:34:A:ALA:HB2	1:105:A:VAL:HB	2	0.11	0.01	0.11
(1,355)	1:34:A:ALA:HB3	1:105:A:VAL:HB	2	0.11	0.01	0.11
(1,444)	1:43:A:LEU:HA	1:46:A:LEU:HB3	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD2	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD3	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD2	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD3	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD2	2	0.11	0.0	0.11
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD3	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD21	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD22	2	0.11	0.0	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD23	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD11	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD12	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD13	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD11	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD12	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD13	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD11	2	0.11	0.0	0.11

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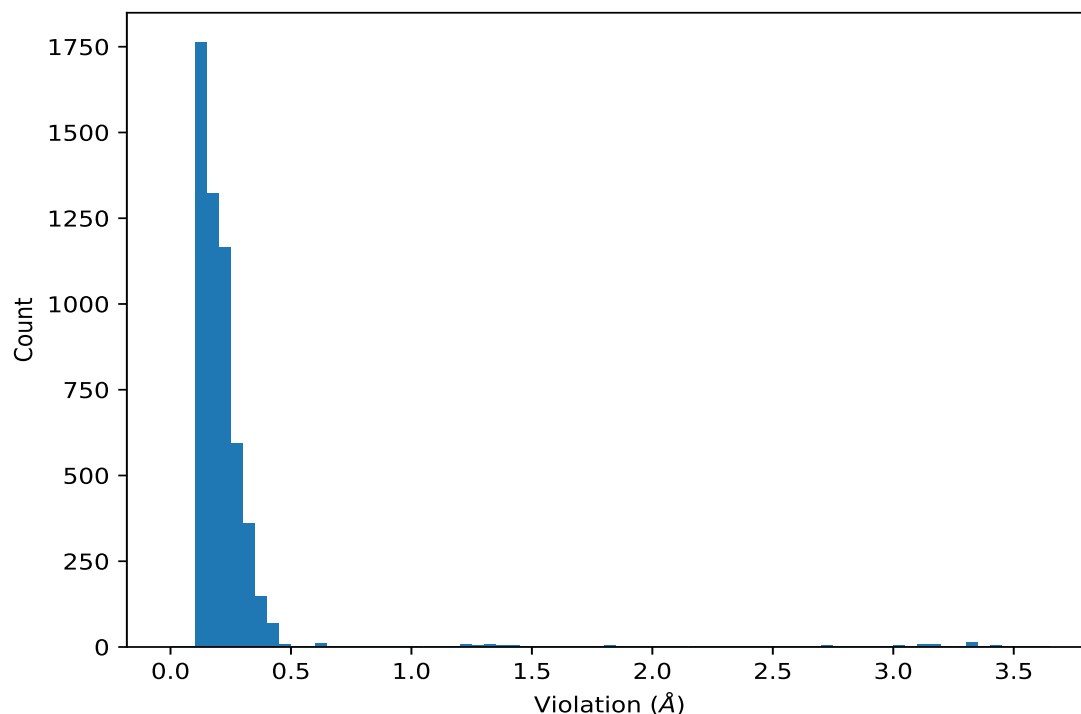
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD12	2	0.11	0.0	0.11
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD13	2	0.11	0.0	0.11
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD2	2	0.11	0.0	0.11
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD3	2	0.11	0.0	0.11
(1,1900)	1:44:A:VAL:HG21	1:46:A:LEU:H	2	0.11	0.0	0.11
(1,1900)	1:44:A:VAL:HG22	1:46:A:LEU:H	2	0.11	0.0	0.11
(1,1900)	1:44:A:VAL:HG23	1:46:A:LEU:H	2	0.11	0.0	0.11
(1,2142)	1:65:A:ILE:HG13	1:65:A:ILE:H	2	0.11	0.0	0.11
(1,2454)	1:83:A:SER:H	1:86:A:ARG:HB2	2	0.11	0.0	0.11
(1,138)	1:17:A:GLU:HG2	1:17:A:GLU:HA	2	0.1	0.0	0.1
(1,2680)	1:93:A:GLU:HG2	1:93:A:GLU:H	2	0.1	0.0	0.1
(1,2687)	1:93:A:GLU:HG2	1:94:A:HIS:H	2	0.1	0.0	0.1
(1,3093)	1:116:A:LEU:HG	1:119:A:PHE:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	8	3.64
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	5	3.58
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	9	3.52
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	7	3.47
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	9	3.42
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	8	3.41
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	8	3.41
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	8	3.41
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	8	3.38
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	5	3.37
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	10	3.34
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	7	3.34
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	2	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	5	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	5	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	5	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	7	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	7	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	7	3.31
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	9	3.3
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	9	3.3
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	9	3.3
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	1	3.2
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	10	3.19
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	10	3.19
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	10	3.19
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	1	3.19
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	6	3.16
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	6	3.16
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	6	3.16
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	6	3.16
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	2	3.13
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	2	3.13
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	2	3.13
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	1	3.11
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	1	3.11
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	1	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	6	3.11
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	10	3.11
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	2	3.08
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	3	3.03
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	3	3.03
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	3	3.03
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	3	3.03
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	3	3.01
(1,2643)	1:91:A:TYR:HE1	1:108:A:ALA:H	4	2.89
(1,3206)	1:91:A:TYR:HE1	1:108:A:ALA:HA	4	2.73
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB1	4	2.72
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB2	4	2.72
(1,3205)	1:91:A:TYR:HE1	1:108:A:ALA:HB3	4	2.72
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	9	1.97
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	8	1.95
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	7	1.93
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	5	1.91
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	1	1.81
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	2	1.8
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	10	1.8
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	6	1.72
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	3	1.58
(1,2642)	1:91:A:TYR:HD1	1:108:A:ALA:H	4	1.58
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	8	1.43
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	8	1.43
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	8	1.43
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	1	1.37
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	1	1.37
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	1	1.37
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	10	1.32
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	10	1.32
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	10	1.32
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	6	1.3
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	6	1.3
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	6	1.3
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	5	1.25
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	5	1.25
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	5	1.25
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	3	1.23
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	3	1.23
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	3	1.23
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	7	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	7	1.22
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	7	1.22
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	10	0.65
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	8	0.6
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	8	0.6
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	8	0.6
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	8	0.6
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	8	0.6
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	8	0.6
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	8	0.6
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	8	0.6
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	8	0.6
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	2	0.57
(1,2163)	1:68:A:LEU:HG	1:68:A:LEU:H	1	0.52
(1,1683)	1:33:A:MET:HB2	1:34:A:ALA:H	4	0.49
(1,2107)	1:60:A:ARG:HB2	1:60:A:ARG:H	7	0.47
(1,1699)	1:33:A:MET:HB3	1:102:A:SER:H	6	0.46
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	5	0.45
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	5	0.45
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	5	0.45
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	7	0.44
(1,2444)	1:83:A:SER:HB3	1:84:A:VAL:H	4	0.44
(1,2444)	1:83:A:SER:HB3	1:84:A:VAL:H	5	0.44
(1,2444)	1:83:A:SER:HB3	1:84:A:VAL:H	9	0.44
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	2	0.44
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	4	0.44
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	8	0.44
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	9	0.44
(1,2009)	1:51:A:ASN:HB2	1:51:A:ASN:HD21	7	0.44
(1,2004)	1:51:A:ASN:HB3	1:51:A:ASN:H	5	0.44
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	9	0.44
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	6	0.44
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	6	0.44
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	6	0.44
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	6	0.44
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	6	0.44
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	6	0.44
(1,291)	1:28:A:GLN:HG2	1:101:A:THR:HA	5	0.44
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	7	0.43
(1,2172)	1:69:A:ILE:HG13	1:69:A:ILE:H	5	0.43
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	8	0.43
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	4	0.43
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	10	0.43
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	10	0.43
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	7	0.43
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	7	0.43
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	7	0.43
(1,2172)	1:69:A:ILE:HG13	1:69:A:ILE:H	8	0.42
(1,2028)	1:51:A:ASN:H	1:53:A:LEU:H	5	0.42
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	9	0.42
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	10	0.42
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	6	0.42
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	6	0.42
(1,995)	1:103:A:LEU:HD11	1:105:A:VAL:HB	8	0.42
(1,995)	1:103:A:LEU:HD12	1:105:A:VAL:HB	8	0.42
(1,995)	1:103:A:LEU:HD13	1:105:A:VAL:HB	8	0.42
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	10	0.42
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	10	0.42
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	10	0.42
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	3	0.41
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	3	0.41
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	3	0.41
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	6	0.41
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	7	0.41
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	1	0.41
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	1	0.41
(1,1343)	1:15:A:THR:HB	1:17:A:GLU:H	8	0.41
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	1	0.41
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	1	0.41
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	1	0.41
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	4	0.41
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	5	0.41
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	7	0.41
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	7	0.4
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	7	0.4
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	7	0.4
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	8	0.4
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	8	0.4
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	8	0.4
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	3	0.4
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	7	0.4
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	8	0.4
(1,1343)	1:15:A:THR:HB	1:17:A:GLU:H	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	3	0.4
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	3	0.4
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	3	0.4
(1,628)	1:65:A:ILE:HG13	1:66:A:SER:HA	7	0.4
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	5	0.39
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	5	0.39
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	5	0.39
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	6	0.39
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	6	0.39
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	6	0.39
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	10	0.39
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	10	0.39
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	10	0.39
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	1	0.39
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	4	0.39
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	2	0.39
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	2	0.39
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	10	0.39
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	5	0.39
(1,1124)	1:114:A:ARG:HA	1:116:A:LEU:HD11	10	0.39
(1,1124)	1:114:A:ARG:HA	1:116:A:LEU:HD12	10	0.39
(1,1124)	1:114:A:ARG:HA	1:116:A:LEU:HD13	10	0.39
(1,991)	1:103:A:LEU:HD11	1:103:A:LEU:HA	8	0.39
(1,991)	1:103:A:LEU:HD12	1:103:A:LEU:HA	8	0.39
(1,991)	1:103:A:LEU:HD13	1:103:A:LEU:HA	8	0.39
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	2	0.39
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	8	0.39
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	9	0.39
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	2	0.38
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	2	0.38
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	2	0.38
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	4	0.38
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	6	0.38
(1,2036)	1:52:A:LEU:HD21	1:52:A:LEU:H	9	0.38
(1,2036)	1:52:A:LEU:HD22	1:52:A:LEU:H	9	0.38
(1,2036)	1:52:A:LEU:HD23	1:52:A:LEU:H	9	0.38
(1,2007)	1:51:A:ASN:HB3	1:51:A:ASN:HD22	4	0.38
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	9	0.38
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	9	0.38
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	1	0.38
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	1	0.38
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	1	0.38
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	1	0.38
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	1	0.38
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	1	0.38
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	1	0.38
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	1	0.38
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	10	0.38
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	2	0.37
(1,3086)	1:116:A:LEU:HA	1:117:A:TYR:H	6	0.37
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	1	0.37
(1,2940)	1:107:A:TYR:HD2	1:108:A:ALA:H	8	0.37
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	1	0.37
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	4	0.37
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	8	0.37
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	10	0.37
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	3	0.37
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	1	0.37
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	10	0.37
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	7	0.37
(1,1893)	1:44:A:VAL:HB	1:45:A:GLY:H	8	0.37
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	5	0.37
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	5	0.37
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	10	0.37
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	10	0.37
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	10	0.37
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	1	0.37
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	1	0.37
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	1	0.37
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	1	0.37
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	3	0.37
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	9	0.36
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	9	0.36
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	9	0.36
(1,3086)	1:116:A:LEU:HA	1:117:A:TYR:H	8	0.36
(1,3077)	1:115:A:THR:HB	1:116:A:LEU:H	8	0.36
(1,2940)	1:107:A:TYR:HD2	1:108:A:ALA:H	2	0.36
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	3	0.36
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	6	0.36
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	3	0.36
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	7	0.36
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	3	0.36
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	9	0.36
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	3	0.36
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	9	0.36
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	5	0.36
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	9	0.36
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	3	0.36
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	6	0.36
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	3	0.36
(1,2252)	1:74:A:ARG:H	1:77:A:LEU:H	5	0.36
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	3	0.36
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	6	0.36
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	4	0.36
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	5	0.36
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	2	0.36
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	2	0.36
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	4	0.36
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	4	0.36
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	4	0.36
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	2	0.36
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	10	0.36
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG11	6	0.36
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG12	6	0.36
(1,677)	1:72:A:GLU:HA	1:76:A:VAL:HG13	6	0.36
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB1	1	0.36
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB2	1	0.36
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB3	1	0.36
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB1	1	0.36
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB2	1	0.36
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB3	1	0.36
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB1	1	0.36
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB2	1	0.36
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB3	1	0.36
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	2	0.36
(1,177)	1:22:A:ASP:HA	1:25:A:LEU:HB3	6	0.36
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	6	0.35
(1,3047)	1:112:A:GLN:HB3	1:113:A:GLY:H	9	0.35
(1,2940)	1:107:A:TYR:HD2	1:108:A:ALA:H	10	0.35
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	8	0.35
(1,2767)	1:98:A:LYS:HD3	1:98:A:LYS:H	10	0.35
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	8	0.35
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	6	0.35
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	1	0.35
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	2	0.35
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	2	0.35
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	5	0.35
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	6	0.35
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	6	0.35
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	9	0.35
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	9	0.35
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	1	0.35
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	5	0.35
(1,2160)	1:68:A:LEU:HB3	1:68:A:LEU:H	1	0.35
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	1	0.35
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	10	0.35
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	3	0.35
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	3	0.35
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	8	0.35
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	8	0.35
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	4	0.35
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	4	0.35
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	5	0.35
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	5	0.35
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	5	0.35
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	6	0.35
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD11	7	0.35
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD12	7	0.35
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD13	7	0.35
(1,3061)	1:114:A:ARG:HG3	1:114:A:ARG:H	9	0.34
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	3	0.34
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	5	0.34
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	6	0.34
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	7	0.34
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	10	0.34
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	3	0.34
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	8	0.34
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	10	0.34
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	2	0.34
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	10	0.34
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	7	0.34
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	10	0.34
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	10	0.34
(1,2364)	1:80:A:PHE:HZ	1:81:A:LEU:H	1	0.34
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	2	0.34
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	10	0.34
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	9	0.34
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	3	0.34
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	1	0.34
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	4	0.34
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	8	0.34
(1,1764)	1:37:A:GLU:HG2	1:37:A:GLU:H	8	0.34
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	4	0.34
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	1	0.34
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	3	0.34
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	5	0.34
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	8	0.34
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	9	0.34
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	6	0.34
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	5	0.34
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	5	0.34
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	5	0.34
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	6	0.34
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	6	0.34
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	6	0.34
(1,1613)	1:30:A:MET:HG2	1:31:A:ALA:H	7	0.34
(1,1613)	1:30:A:MET:HG3	1:31:A:ALA:H	7	0.34
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	9	0.34
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	7	0.34
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	7	0.34
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	7	0.34
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	3	0.34
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	7	0.34
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	8	0.34
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	10	0.34
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	10	0.34
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	10	0.34
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	1	0.34
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	3	0.34
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	7	0.34
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	9	0.34
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	9	0.34
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	9	0.34
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	9	0.34
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	9	0.34
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	8	0.34
(1,409)	1:41:A:ALA:HA	1:44:A:VAL:HG21	8	0.34
(1,409)	1:41:A:ALA:HA	1:44:A:VAL:HG22	8	0.34
(1,409)	1:41:A:ALA:HA	1:44:A:VAL:HG23	8	0.34
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	3	0.34
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	4	0.34
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	3	0.33
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	7	0.33
(1,2940)	1:107:A:TYR:HD2	1:108:A:ALA:H	5	0.33
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	1	0.33
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	2	0.33
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	4	0.33
(1,2707)	1:94:A:HIS:HA	1:95:A:ALA:H	9	0.33
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	1	0.33
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	2	0.33
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	7	0.33
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	2	0.33
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	3	0.33
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	7	0.33
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	10	0.33
(1,2464)	1:84:A:VAL:H	1:85:A:ILE:HG12	7	0.33
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	4	0.33
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	1	0.33
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	5	0.33
(1,2249)	1:74:A:ARG:HB2	1:76:A:VAL:H	4	0.33
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	7	0.33
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	10	0.33
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	3	0.33
(1,2026)	1:51:A:ASN:HB3	1:53:A:LEU:H	7	0.33
(1,1996)	1:50:A:THR:HB	1:50:A:THR:H	9	0.33
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	2	0.33
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	4	0.33
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	7	0.33
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	4	0.33
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	3	0.33
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	3	0.33
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	3	0.33
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	6	0.33
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	6	0.33
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	6	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	2	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	2	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	6	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	6	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	6	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	9	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	9	0.33
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	9	0.33
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	6	0.33
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	5	0.33
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	8	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	1	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	2	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	3	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	4	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	5	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	6	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	7	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	8	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	9	0.33
(1,769)	1:78:A:LYS:HE2	1:78:A:LYS:HB2	10	0.33
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	4	0.33
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	4	0.33
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	4	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	4	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	4	0.33
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	4	0.33
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB1	5	0.33
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB2	5	0.33
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB3	5	0.33
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB1	5	0.33
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB2	5	0.33
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB3	5	0.33
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB1	5	0.33
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB2	5	0.33
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB3	5	0.33
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	9	0.32
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	6	0.32
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	5	0.32
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	5	0.32
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	7	0.32
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	8	0.32
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	5	0.32
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	6	0.32
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	3	0.32
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	7	0.32
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	7	0.32
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	8	0.32
(1,2139)	1:64:A:ARG:H	1:65:A:ILE:H	9	0.32
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	5	0.32
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	9	0.32
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	5	0.32
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	1	0.32
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	2	0.32
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	8	0.32
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	6	0.32
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	6	0.32
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	6	0.32
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	4	0.32
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	4	0.32
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	2	0.32
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	2	0.32
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	2	0.32
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	4	0.32
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	4	0.32
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	4	0.32
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	5	0.32
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	5	0.32
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	5	0.32
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	2	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	7	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	7	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	7	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	8	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	8	0.32
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	8	0.32
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	1	0.32
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	7	0.32
(1,829)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	1	0.32
(1,829)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	1	0.32
(1,829)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	1	0.32
(1,624)	1:65:A:ILE:HA	1:65:A:ILE:HG12	3	0.32
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	7	0.32
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	4	0.31
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	8	0.31
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	2	0.31
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	3	0.31
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	9	0.31
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	6	0.31
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	4	0.31
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	4	0.31
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	5	0.31
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	9	0.31
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	2	0.31
(1,2249)	1:74:A:ARG:HB2	1:76:A:VAL:H	2	0.31
(1,2139)	1:64:A:ARG:H	1:65:A:ILE:H	3	0.31
(1,2000)	1:50:A:THR:HB	1:51:A:ASN:H	3	0.31
(1,1968)	1:48:A:GLU:HG3	1:48:A:GLU:H	1	0.31
(1,1968)	1:48:A:GLU:HG3	1:48:A:GLU:H	6	0.31
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	8	0.31
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	2	0.31
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	3	0.31
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	6	0.31
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	7	0.31
(1,1764)	1:37:A:GLU:HG2	1:37:A:GLU:H	1	0.31
(1,1694)	1:33:A:MET:H	1:36:A:GLN:HE21	6	0.31
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	9	0.31
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	2	0.31
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	10	0.31
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	2	0.31
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	2	0.31
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	2	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	1	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	2	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	5	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	6	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	8	0.31
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	9	0.31
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	8	0.31
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	8	0.31
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	8	0.31
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	1	0.31
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	4	0.31
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	5	0.31
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	9	0.31
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	2	0.31
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	2	0.31
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	3	0.31
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	3	0.31
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	3	0.31
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	3	0.31
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD11	1	0.31
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD12	1	0.31
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD13	1	0.31
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	8	0.31
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	8	0.31
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	8	0.31
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	8	0.31
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	8	0.31
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	8	0.31
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	8	0.31
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	8	0.31
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	8	0.31
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	8	0.31
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	8	0.31
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	8	0.31
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	8	0.31
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	6	0.31
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	2	0.31
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	2	0.31
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	2	0.31
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	10	0.31
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	10	0.31
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	10	0.31
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	1	0.31
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	1	0.31
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	1	0.31
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	1	0.31
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	1	0.31
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	1	0.31
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	1	0.31
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	1	0.31
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	1	0.31
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	1	0.31
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	1	0.31
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	2	0.31
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	2	0.31
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	2	0.31
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	5	0.31
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	5	0.31
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	5	0.31
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	4	0.3
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	1	0.3
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	1	0.3
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	1	0.3
(1,3129)	1:14:A:VAL:HG21	1:18:A:PHE:HD2	4	0.3
(1,3129)	1:14:A:VAL:HG22	1:18:A:PHE:HD2	4	0.3
(1,3129)	1:14:A:VAL:HG23	1:18:A:PHE:HD2	4	0.3
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	1	0.3
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	4	0.3
(1,2837)	1:103:A:LEU:HB3	1:103:A:LEU:H	7	0.3
(1,2749)	1:97:A:ARG:HG2	1:97:A:ARG:HE	2	0.3
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	1	0.3
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	10	0.3
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	3	0.3
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	7	0.3
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	8	0.3
(1,2541)	1:87:A:ASP:HA	1:88:A:SER:H	9	0.3
(1,2501)	1:85:A:ILE:H	1:87:A:ASP:H	8	0.3
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	1	0.3
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	2	0.3
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	5	0.3
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	8	0.3
(1,2353)	1:79:A:SER:HB2	1:83:A:SER:H	10	0.3
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	9	0.3
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	10	0.3
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	3	0.3
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	6	0.3
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	9	0.3
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	9	0.3
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	9	0.3
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	1	0.3
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	2	0.3
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	4	0.3
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	6	0.3
(1,1828)	1:41:A:ALA:H	1:43:A:LEU:H	9	0.3
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	8	0.3
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	9	0.3
(1,1370)	1:17:A:GLU:HG3	1:17:A:GLU:H	3	0.3
(1,1344)	1:15:A:THR:H	1:17:A:GLU:HG2	4	0.3
(1,1344)	1:15:A:THR:H	1:17:A:GLU:HG2	10	0.3
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	8	0.3
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	6	0.3
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	6	0.3
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	6	0.3
(1,707)	1:74:A:ARG:HD2	1:74:A:ARG:HB3	1	0.3
(1,707)	1:74:A:ARG:HD2	1:74:A:ARG:HB3	5	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	1	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	1	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	1	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	3	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	3	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	3	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	10	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	10	0.3
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	10	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	1	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	1	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	1	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	3	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	3	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	3	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	4	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	4	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	4	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	5	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	5	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	5	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	7	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	7	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	7	0.3
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	8	0.3
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	8	0.3
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	8	0.3
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	8	0.3
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	4	0.3
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	4	0.3
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	6	0.3
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	6	0.3
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	6	0.3
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	9	0.3
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	9	0.3
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	9	0.3
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG11	8	0.3
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG12	8	0.3
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG13	8	0.3
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	10	0.29
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	5	0.29
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	6	0.29
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	1	0.29
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	3	0.29
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	2	0.29
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	3	0.29
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	3	0.29
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	4	0.29
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	6	0.29
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	10	0.29
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	4	0.29
(1,2249)	1:74:A:ARG:HB2	1:76:A:VAL:H	10	0.29
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	2	0.29
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	2	0.29
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	2	0.29
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	1	0.29
(1,2134)	1:64:A:ARG:HB2	1:64:A:ARG:H	3	0.29
(1,2065)	1:55:A:LEU:HD21	1:55:A:LEU:H	9	0.29
(1,2065)	1:55:A:LEU:HD22	1:55:A:LEU:H	9	0.29
(1,2065)	1:55:A:LEU:HD23	1:55:A:LEU:H	9	0.29
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	5	0.29
(1,2008)	1:51:A:ASN:HA	1:51:A:ASN:HD22	7	0.29
(1,2004)	1:51:A:ASN:HB3	1:51:A:ASN:H	2	0.29
(1,1968)	1:48:A:GLU:HG3	1:48:A:GLU:H	8	0.29
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	9	0.29
(1,1681)	1:33:A:MET:HG2	1:33:A:MET:H	4	0.29
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	4	0.29
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	3	0.29
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	3	0.29
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	3	0.29
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	7	0.29
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	7	0.29
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	8	0.29
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	8	0.29
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	8	0.29
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	1	0.29
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	5	0.29
(1,1344)	1:15:A:THR:H	1:17:A:GLU:HG2	7	0.29
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	1	0.29
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	1	0.29
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	1	0.29
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	3	0.29
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	4	0.29
(1,1230)	1:10:A:LEU:HB3	1:11:A:VAL:H	10	0.29
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG11	3	0.29
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG12	3	0.29
(1,1007)	1:104:A:ASP:HA	1:106:A:VAL:HG13	3	0.29
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	4	0.29
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	9	0.29
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	4	0.29
(1,707)	1:74:A:ARG:HD2	1:74:A:ARG:HB3	3	0.29
(1,707)	1:74:A:ARG:HD2	1:74:A:ARG:HB3	6	0.29
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	10	0.29
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	10	0.29
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	10	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	2	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	2	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	2	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	4	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	4	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	4	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	7	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	7	0.29
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	7	0.29
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	1	0.29
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	10	0.29
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	6	0.29
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	6	0.29
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	6	0.29
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB1	3	0.29
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB2	3	0.29
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB3	3	0.29
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB1	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB2	3	0.29
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB3	3	0.29
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB1	3	0.29
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB2	3	0.29
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB3	3	0.29
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	8	0.29
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	7	0.29
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	2	0.29
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	2	0.29
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	2	0.29
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	2	0.29
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	2	0.29
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	2	0.29
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	2	0.29
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	2	0.29
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	2	0.29
(1,58)	1:10:A:LEU:HD21	1:10:A:LEU:HA	10	0.29
(1,58)	1:10:A:LEU:HD22	1:10:A:LEU:HA	10	0.29
(1,58)	1:10:A:LEU:HD23	1:10:A:LEU:HA	10	0.29
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	1	0.28
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	5	0.28
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	1	0.28
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	4	0.28
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	10	0.28
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	8	0.28
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	3	0.28
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	3	0.28
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	3	0.28
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	10	0.28
(1,3023)	1:111:A:ARG:HG3	1:112:A:GLN:H	6	0.28
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	6	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	1	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	3	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	7	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	8	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	9	0.28
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	10	0.28
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	4	0.28
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	4	0.28
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	4	0.28
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	1	0.28
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	9	0.28
(1,2748)	1:97:A:ARG:HG3	1:97:A:ARG:HE	1	0.28
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	2	0.28
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	6	0.28
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	9	0.28
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	10	0.28
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	4	0.28
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	7	0.28
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	6	0.28
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	10	0.28
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	4	0.28
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	7	0.28
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	9	0.28
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	1	0.28
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	5	0.28
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	7	0.28
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	7	0.28
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	8	0.28
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	8	0.28
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	3	0.28
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	3	0.28
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	3	0.28
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	5	0.28
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	1	0.28
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	4	0.28
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	8	0.28
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	10	0.28
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	2	0.28
(1,1683)	1:33:A:MET:HB2	1:34:A:ALA:H	6	0.28
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	8	0.28
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	9	0.28
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	9	0.28
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	9	0.28
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	3	0.28
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	7	0.28
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	1	0.28
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	7	0.28
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	8	0.28
(1,1456)	1:22:A:ASP:HB3	1:24:A:ASP:H	10	0.28
(1,1331)	1:14:A:VAL:HG11	1:82:A:GLU:H	9	0.28
(1,1331)	1:14:A:VAL:HG12	1:82:A:GLU:H	9	0.28
(1,1331)	1:14:A:VAL:HG13	1:82:A:GLU:H	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	2	0.28
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	6	0.28
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	10	0.28
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	10	0.28
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	1	0.28
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	7	0.28
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	8	0.28
(1,890)	1:89:A:VAL:HG21	1:100:A:VAL:HA	4	0.28
(1,890)	1:89:A:VAL:HG22	1:100:A:VAL:HA	4	0.28
(1,890)	1:89:A:VAL:HG23	1:100:A:VAL:HA	4	0.28
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	7	0.28
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	7	0.28
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	7	0.28
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	7	0.28
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	7	0.28
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	7	0.28
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	7	0.28
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	7	0.28
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	7	0.28
(1,884)	1:89:A:VAL:HA	1:92:A:THR:HB	9	0.28
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	7	0.28
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	7	0.28
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	7	0.28
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	8	0.28
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	8	0.28
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	8	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	5	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	5	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	5	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD21	6	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD22	6	0.28
(1,557)	1:55:A:LEU:HA	1:55:A:LEU:HD23	6	0.28
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB1	9	0.28
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB2	9	0.28
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB3	9	0.28
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB1	9	0.28
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB2	9	0.28
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB3	9	0.28
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB1	9	0.28
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB2	9	0.28
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB3	9	0.28
(1,473)	1:46:A:LEU:HD11	1:46:A:LEU:HA	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:46:A:LEU:HD12	1:46:A:LEU:HA	9	0.28
(1,473)	1:46:A:LEU:HD13	1:46:A:LEU:HA	9	0.28
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	9	0.28
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	3	0.28
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	6	0.28
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	8	0.28
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	10	0.28
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG11	9	0.28
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG12	9	0.28
(1,29)	1:8:A:ALA:HA	1:11:A:VAL:HG13	9	0.28
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB1	2	0.28
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB2	2	0.28
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB3	2	0.28
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	1	0.27
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	2	0.27
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	3	0.27
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	6	0.27
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	9	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	2	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	5	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	6	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	7	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	8	0.27
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	9	0.27
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	5	0.27
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	2	0.27
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	2	0.27
(1,3013)	1:111:A:ARG:HB2	1:111:A:ARG:H	4	0.27
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	3	0.27
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	1	0.27
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	1	0.27
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	1	0.27
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	3	0.27
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	3	0.27
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	3	0.27
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	9	0.27
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	9	0.27
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	9	0.27
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	3	0.27
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	4	0.27
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	8	0.27
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	5	0.27
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	7	0.27
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	9	0.27
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	1	0.27
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	8	0.27
(1,2592)	1:89:A:VAL:HA	1:93:A:GLU:H	4	0.27
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	5	0.27
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	1	0.27
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	5	0.27
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	6	0.27
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	2	0.27
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	2	0.27
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	5	0.27
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	7	0.27
(1,2491)	1:85:A:ILE:HG12	1:85:A:ILE:H	9	0.27
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	1	0.27
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	5	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	1	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	2	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	3	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	4	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	5	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	6	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	7	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	9	0.27
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	10	0.27
(1,2284)	1:76:A:VAL:H	1:79:A:SER:HB3	8	0.27
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	6	0.27
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	6	0.27
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	6	0.27
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	7	0.27
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	7	0.27
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	7	0.27
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	8	0.27
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	8	0.27
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	8	0.27
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	3	0.27
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	9	0.27
(1,2204)	1:72:A:GLU:HB3	1:74:A:ARG:H	9	0.27
(1,2168)	1:68:A:LEU:H	1:72:A:GLU:H	1	0.27
(1,1968)	1:48:A:GLU:HG3	1:48:A:GLU:H	10	0.27
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	7	0.27
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	1	0.27
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	3	0.27
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	2	0.27
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	7	0.27
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	1	0.27
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	2	0.27
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	2	0.27
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	2	0.27
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	6	0.27
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	3	0.27
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	4	0.27
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	5	0.27
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	6	0.27
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	4	0.27
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	8	0.27
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	6	0.27
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	9	0.27
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	7	0.27
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	9	0.27
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	1	0.27
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	1	0.27
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	10	0.27
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	1	0.27
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	1	0.27
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	1	0.27
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	4	0.27
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	4	0.27
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	4	0.27
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	9	0.27
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	9	0.27
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	9	0.27
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	8	0.27
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	8	0.27
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	8	0.27
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	5	0.27
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	6	0.27
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	2	0.27
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	2	0.27
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	2	0.27
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	4	0.27
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	4	0.27
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	2	0.27
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	8	0.27
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	8	0.27
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	8	0.27
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	1	0.27
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	1	0.27
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	4	0.27
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	4	0.26
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	7	0.26
(1,3137)	1:18:A:PHE:HB3	1:18:A:PHE:HZ	3	0.26
(1,3086)	1:116:A:LEU:HA	1:117:A:TYR:H	10	0.26
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	7	0.26
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	7	0.26
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	7	0.26
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	3	0.26
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	3	0.26
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	8	0.26
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	9	0.26
(1,3017)	1:111:A:ARG:H	1:112:A:GLN:HB3	9	0.26
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	6	0.26
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	8	0.26
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	7	0.26
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	7	0.26
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	7	0.26
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	2	0.26
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	5	0.26
(1,2820)	1:102:A:SER:HA	1:103:A:LEU:H	10	0.26
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	10	0.26
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	2	0.26
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	3	0.26
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	4	0.26
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	5	0.26
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	10	0.26
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	8	0.26
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	5	0.26
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	9	0.26
(1,2516)	1:86:A:ARG:HG2	1:86:A:ARG:H	10	0.26
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	4	0.26
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	3	0.26
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	6	0.26
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	8	0.26
(1,2311)	1:78:A:LYS:HG3	1:78:A:LYS:H	8	0.26
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	7	0.26
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	1	0.26
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	1	0.26
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	1	0.26
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	4	0.26
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	4	0.26
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	4	0.26
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	5	0.26
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	5	0.26
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	5	0.26
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	6	0.26
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	7	0.26
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	3	0.26
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	5	0.26
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	9	0.26
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	5	0.26
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	6	0.26
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	4	0.26
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	5	0.26
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	9	0.26
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	4	0.26
(1,1477)	1:23:A:GLN:HB2	1:24:A:ASP:H	2	0.26
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	5	0.26
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	2	0.26
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	10	0.26
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	4	0.26
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	5	0.26
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	4	0.26
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	4	0.26
(1,1110)	1:113:A:GLY:HA2	1:114:A:ARG:HG3	9	0.26
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	5	0.26
(1,1086)	1:110:A:LYS:HE2	1:110:A:LYS:HB2	1	0.26
(1,1086)	1:110:A:LYS:HE3	1:110:A:LYS:HB2	1	0.26
(1,1086)	1:110:A:LYS:HE2	1:110:A:LYS:HB2	6	0.26
(1,1086)	1:110:A:LYS:HE3	1:110:A:LYS:HB2	6	0.26
(1,1086)	1:110:A:LYS:HE2	1:110:A:LYS:HB2	8	0.26
(1,1086)	1:110:A:LYS:HE3	1:110:A:LYS:HB2	8	0.26
(1,1086)	1:110:A:LYS:HE2	1:110:A:LYS:HB2	10	0.26
(1,1086)	1:110:A:LYS:HE3	1:110:A:LYS:HB2	10	0.26
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	3	0.26
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	3	0.26
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	5	0.26
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	5	0.26
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	5	0.26
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	7	0.26
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	7	0.26
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	7	0.26
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	8	0.26
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	8	0.26
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	8	0.26
(1,995)	1:103:A:LEU:HD11	1:105:A:VAL:HB	2	0.26
(1,995)	1:103:A:LEU:HD12	1:105:A:VAL:HB	2	0.26
(1,995)	1:103:A:LEU:HD13	1:105:A:VAL:HB	2	0.26
(1,995)	1:103:A:LEU:HD11	1:105:A:VAL:HB	5	0.26
(1,995)	1:103:A:LEU:HD12	1:105:A:VAL:HB	5	0.26
(1,995)	1:103:A:LEU:HD13	1:105:A:VAL:HB	5	0.26
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	5	0.26
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	5	0.26
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	5	0.26
(1,631)	1:65:A:ILE:HG21	1:68:A:LEU:HA	9	0.26
(1,631)	1:65:A:ILE:HG22	1:68:A:LEU:HA	9	0.26
(1,631)	1:65:A:ILE:HG23	1:68:A:LEU:HA	9	0.26
(1,546)	1:53:A:LEU:HD21	1:57:A:LEU:HB2	6	0.26
(1,546)	1:53:A:LEU:HD22	1:57:A:LEU:HB2	6	0.26
(1,546)	1:53:A:LEU:HD23	1:57:A:LEU:HB2	6	0.26
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	3	0.26
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	5	0.26
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	8	0.26
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	9	0.26
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	9	0.26
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	9	0.26
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	4	0.26
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	4	0.26
(1,163)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	4	0.26
(1,163)	1:21:A:LYS:HE3	1:21:A:LYS:HB3	4	0.26
(1,163)	1:21:A:LYS:HE2	1:21:A:LYS:HB3	9	0.26
(1,163)	1:21:A:LYS:HE3	1:21:A:LYS:HB3	9	0.26
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	6	0.26
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	4	0.25
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	8	0.25
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	6	0.25
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	7	0.25
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	1	0.25
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	4	0.25
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	7	0.25
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	10	0.25
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	10	0.25
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	2	0.25
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	5	0.25
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	2	0.25
(1,2757)	1:97:A:ARG:HB3	1:98:A:LYS:H	1	0.25
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	7	0.25
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	7	0.25
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	9	0.25
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	5	0.25
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	8	0.25
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	2	0.25
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG21	4	0.25
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG22	4	0.25
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG23	4	0.25
(1,2488)	1:85:A:ILE:HG13	1:85:A:ILE:H	1	0.25
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	9	0.25
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	2	0.25
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	4	0.25
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	5	0.25
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	10	0.25
(1,2378)	1:80:A:PHE:H	1:84:A:VAL:H	8	0.25
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	1	0.25
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	6	0.25
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	1	0.25
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	1	0.25
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	8	0.25
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	9	0.25
(1,2141)	1:65:A:ILE:HG12	1:65:A:ILE:H	6	0.25
(1,1794)	1:39:A:SER:HB2	1:39:A:SER:H	2	0.25
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	5	0.25
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	6	0.25
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	1	0.25
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	6	0.25
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	5	0.25
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	8	0.25
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	2	0.25
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	9	0.25
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	9	0.25
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	10	0.25
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	3	0.25
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	7	0.25
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	5	0.25
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	1	0.25
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	6	0.25
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	2	0.25
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	2	0.25
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	2	0.25
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	4	0.25
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	4	0.25
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	4	0.25
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	10	0.25
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	10	0.25
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	10	0.25
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	7	0.25
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	7	0.25
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	7	0.25
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	8	0.25
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	8	0.25
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	8	0.25
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	7	0.25
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	7	0.25
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	7	0.25
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	7	0.25
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	7	0.25
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	7	0.25
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	7	0.25
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	7	0.25
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	7	0.25
(1,995)	1:103:A:LEU:HD11	1:105:A:VAL:HB	10	0.25
(1,995)	1:103:A:LEU:HD12	1:105:A:VAL:HB	10	0.25
(1,995)	1:103:A:LEU:HD13	1:105:A:VAL:HB	10	0.25
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	2	0.25
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	2	0.25
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	5	0.25
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	5	0.25
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	5	0.25
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	5	0.25
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	5	0.25
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	5	0.25
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	5	0.25
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	5	0.25
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	8	0.25
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	8	0.25
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	8	0.25
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	5	0.25
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	9	0.25
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD11	10	0.25
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD12	10	0.25
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD13	10	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	3	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	3	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	3	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	3	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	3	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	3	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	3	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	3	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	3	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	5	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	5	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	5	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	5	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	5	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	5	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	5	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	5	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	5	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	10	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	10	0.25
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	10	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	10	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	10	0.25
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	10	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	10	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	10	0.25
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	10	0.25
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	2	0.25
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	2	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	2	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	2	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	2	0.25
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	7	0.25
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	7	0.25
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	7	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	7	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	7	0.25
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	7	0.25
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	1	0.25
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	3	0.25
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	6	0.25
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	6	0.25
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	6	0.25
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	5	0.24
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	8	0.24
(1,3153)	1:27:A:TRP:HB2	1:27:A:TRP:HE3	8	0.24
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	1	0.24
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	4	0.24
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	9	0.24
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	1	0.24
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	5	0.24
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	8	0.24
(1,3020)	1:111:A:ARG:HA	1:112:A:GLN:H	5	0.24
(1,3010)	1:110:A:LYS:HB2	1:116:A:LEU:H	10	0.24
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	2	0.24
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	4	0.24
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	9	0.24
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	10	0.24
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	10	0.24
(1,2854)	1:103:A:LEU:HD21	1:105:A:VAL:H	6	0.24
(1,2854)	1:103:A:LEU:HD22	1:105:A:VAL:H	6	0.24
(1,2854)	1:103:A:LEU:HD23	1:105:A:VAL:H	6	0.24
(1,2718)	1:95:A:ALA:H	1:96:A:LYS:HA	8	0.24
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	5	0.24
(1,2634)	1:91:A:TYR:HB2	1:94:A:HIS:H	6	0.24
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	7	0.24
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	4	0.24
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	1	0.24
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	2	0.24
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	6	0.24
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	7	0.24
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	7	0.24
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	3	0.24
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	5	0.24
(1,2434)	1:82:A:GLU:H	1:85:A:ILE:HG13	1	0.24
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	4	0.24
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	1	0.24
(1,2414)	1:82:A:GLU:HG3	1:82:A:GLU:H	9	0.24
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	5	0.24
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	10	0.24
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	5	0.24
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	5	0.24
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	6	0.24
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	6	0.24
(1,2218)	1:73:A:VAL:HG21	1:74:A:ARG:H	10	0.24
(1,2218)	1:73:A:VAL:HG22	1:74:A:ARG:H	10	0.24
(1,2218)	1:73:A:VAL:HG23	1:74:A:ARG:H	10	0.24
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	2	0.24
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	8	0.24
(1,2090)	1:57:A:LEU:HG	1:58:A:VAL:H	8	0.24
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	2	0.24
(1,2000)	1:50:A:THR:HB	1:51:A:ASN:H	8	0.24
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	3	0.24
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	4	0.24
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	7	0.24
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	2	0.24
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	4	0.24
(1,1940)	1:46:A:LEU:H	1:49:A:HIS:H	3	0.24
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	9	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	1	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	2	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	3	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	4	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	6	0.24
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	10	0.24
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	10	0.24
(1,1756)	1:36:A:GLN:H	1:38:A:ALA:H	10	0.24
(1,1748)	1:36:A:GLN:HG3	1:36:A:GLN:H	6	0.24
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	6	0.24
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	4	0.24
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	10	0.24
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	10	0.24
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	8	0.24
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	10	0.24
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	10	0.24
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	10	0.24
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	10	0.24
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	3	0.24
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	9	0.24
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	2	0.24
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	9	0.24
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	1	0.24
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	1	0.24
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	6	0.24
(1,1296)	1:13:A:GLU:HG3	1:13:A:GLU:H	9	0.24
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	2	0.24
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	3	0.24
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	10	0.24
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	10	0.24
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	9	0.24
(1,1083)	1:110:A:LYS:HB2	1:110:A:LYS:HE2	7	0.24
(1,1083)	1:110:A:LYS:HB2	1:110:A:LYS:HE3	7	0.24
(1,1083)	1:110:A:LYS:HB3	1:110:A:LYS:HE2	7	0.24
(1,1083)	1:110:A:LYS:HB3	1:110:A:LYS:HE3	7	0.24
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	1	0.24
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	1	0.24
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	1	0.24
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	6	0.24
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	6	0.24
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	6	0.24
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	2	0.24
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	2	0.24
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	2	0.24
(1,853)	1:85:A:ILE:HA	1:85:A:ILE:HD11	1	0.24
(1,853)	1:85:A:ILE:HA	1:85:A:ILE:HD12	1	0.24
(1,853)	1:85:A:ILE:HA	1:85:A:ILE:HD13	1	0.24
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	9	0.24
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	9	0.24
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	9	0.24
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	9	0.24
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	9	0.24
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	9	0.24
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	9	0.24
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	9	0.24
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	1	0.24
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	1	0.24
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	1	0.24
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	2	0.24
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	2	0.24
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	2	0.24
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	1	0.24
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	1	0.24
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	1	0.24
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	2	0.24
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	2	0.24
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	2	0.24
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	9	0.24
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	9	0.24
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	9	0.24
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	2	0.24
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	4	0.24
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	6	0.24
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	9	0.24
(1,528)	1:52:A:LEU:HG	1:52:A:LEU:HA	5	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	6	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	6	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	6	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	10	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	10	0.24
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	10	0.24
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD11	8	0.24
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD12	8	0.24
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD13	8	0.24
(1,282)	1:28:A:GLN:HG3	1:99:A:THR:HA	8	0.24
(1,212)	1:25:A:LEU:HB3	1:98:A:LYS:HB2	2	0.24
(1,186)	1:23:A:GLN:HG2	1:23:A:GLN:HA	2	0.24
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	1	0.24
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	1	0.24
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	6	0.24
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	6	0.24
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	6	0.24
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	6	0.24
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	6	0.24
(1,5)	1:4:A:LYS:HA	1:4:A:LYS:HD2	4	0.24
(1,5)	1:4:A:LYS:HA	1:4:A:LYS:HD3	4	0.24
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	9	0.23
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	5	0.23
(1,3159)	1:27:A:TRP:HD1	1:99:A:THR:HG21	8	0.23
(1,3159)	1:27:A:TRP:HD1	1:99:A:THR:HG22	8	0.23
(1,3159)	1:27:A:TRP:HD1	1:99:A:THR:HG23	8	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	2	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	3	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	5	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	6	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	7	0.23
(1,3138)	1:18:A:PHE:HB2	1:18:A:PHE:HZ	10	0.23
(1,3062)	1:114:A:ARG:HG2	1:114:A:ARG:H	9	0.23
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	8	0.23
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	1	0.23
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	3	0.23
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	8	0.23
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	8	0.23
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	7	0.23
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	4	0.23
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	3	0.23
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	6	0.23
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	9	0.23
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	4	0.23
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	4	0.23
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	5	0.23
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	8	0.23
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	9	0.23
(1,2540)	1:87:A:ASP:HB3	1:87:A:ASP:H	10	0.23
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	1	0.23
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	4	0.23
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	7	0.23
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	2	0.23
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	2	0.23
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	2	0.23
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	3	0.23
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	6	0.23
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	7	0.23
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	8	0.23
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2248)	1:74:A:ARG:HG2	1:76:A:VAL:H	3	0.23
(1,2248)	1:74:A:ARG:HG3	1:76:A:VAL:H	3	0.23
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	10	0.23
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	8	0.23
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	10	0.23
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	7	0.23
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	10	0.23
(1,2095)	1:58:A:VAL:HG11	1:58:A:VAL:H	4	0.23
(1,2095)	1:58:A:VAL:HG12	1:58:A:VAL:H	4	0.23
(1,2095)	1:58:A:VAL:HG13	1:58:A:VAL:H	4	0.23
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	6	0.23
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	6	0.23
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	6	0.23
(1,2037)	1:52:A:LEU:HB2	1:52:A:LEU:H	5	0.23
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	3	0.23
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	6	0.23
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	8	0.23
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	10	0.23
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	5	0.23
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	4	0.23
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	7	0.23
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	1	0.23
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	2	0.23
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	4	0.23
(1,1721)	1:35:A:LEU:HG	1:35:A:LEU:H	4	0.23
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	4	0.23
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	7	0.23
(1,1585)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	5	0.23
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	1	0.23
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	3	0.23
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	6	0.23
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	10	0.23
(1,1578)	1:28:A:GLN:HG2	1:28:A:GLN:H	5	0.23
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	3	0.23
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	6	0.23
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	9	0.23
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	8	0.23
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	8	0.23
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	8	0.23
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	1	0.23
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	5	0.23
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	10	0.23
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	3	0.23
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	5	0.23
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	6	0.23
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	10	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	1	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	4	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	5	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	7	0.23
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	9	0.23
(1,1240)	1:10:A:LEU:HB2	1:13:A:GLU:H	2	0.23
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	5	0.23
(1,1133)	1:116:A:LEU:HA	1:116:A:LEU:HG	10	0.23
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	4	0.23
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	9	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	1	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	1	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	1	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	1	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	1	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	1	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	1	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	1	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	1	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	6	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	6	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	6	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	6	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	6	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	6	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	6	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	6	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	6	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	8	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	8	0.23
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	8	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	8	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	8	0.23
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	8	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	8	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	8	0.23
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	9	0.23
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	9	0.23
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	9	0.23
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	2	0.23
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	5	0.23
(1,967)	1:98:A:LYS:HA	1:98:A:LYS:HG3	2	0.23
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	7	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	1	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	2	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	3	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	8	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	9	0.23
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	10	0.23
(1,890)	1:89:A:VAL:HG21	1:100:A:VAL:HA	9	0.23
(1,890)	1:89:A:VAL:HG22	1:100:A:VAL:HA	9	0.23
(1,890)	1:89:A:VAL:HG23	1:100:A:VAL:HA	9	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	3	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	3	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	3	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	3	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	3	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	3	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	3	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	3	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	3	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	5	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	5	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	5	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	5	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	5	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	5	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	5	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	5	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	5	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	10	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	10	0.23
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	10	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	10	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	10	0.23
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	10	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	10	0.23
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	10	0.23
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	10	0.23
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	10	0.23
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	10	0.23
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	10	0.23
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	10	0.23
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	10	0.23
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	10	0.23
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	10	0.23
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	10	0.23
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	3	0.23
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	3	0.23
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	3	0.23
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	6	0.23
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	6	0.23
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	6	0.23
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	10	0.23
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	10	0.23
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	10	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	1	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	1	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	1	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	1	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	1	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	1	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	6	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	6	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	6	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	6	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	6	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	6	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	10	0.23
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	10	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	10	0.23
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	10	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	10	0.23
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	10	0.23
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	3	0.23
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	3	0.23
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	3	0.23
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	4	0.23
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	4	0.23
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	5	0.23
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	5	0.23
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	5	0.23
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	6	0.23
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	6	0.23
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	6	0.23
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	5	0.23
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	5	0.23
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	5	0.23
(1,639)	1:68:A:LEU:HD11	1:68:A:LEU:HA	1	0.23
(1,639)	1:68:A:LEU:HD12	1:68:A:LEU:HA	1	0.23
(1,639)	1:68:A:LEU:HD13	1:68:A:LEU:HA	1	0.23
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	7	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	2	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	2	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	2	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	3	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	3	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	3	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	7	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	7	0.23
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	7	0.23
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB1	5	0.23
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB2	5	0.23
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB3	5	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB1	5	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB2	5	0.23
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB3	5	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB1	5	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB2	5	0.23
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB3	5	0.23
(1,313)	1:31:A:ALA:HA	1:33:A:MET:HB2	4	0.23
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	8	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	1	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	1	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	1	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	1	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	1	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	1	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	4	0.23
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	4	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	4	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	4	0.23
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	4	0.23
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB1	10	0.23
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB2	10	0.23
(1,20)	1:7:A:PHE:HB3	1:8:A:ALA:HB3	10	0.23
(1,6)	1:4:A:LYS:HE2	1:4:A:LYS:HB3	4	0.23
(1,6)	1:4:A:LYS:HE3	1:4:A:LYS:HB3	4	0.23
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	2	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	2	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	2	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	8	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	8	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	8	0.22
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	9	0.22
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	1	0.22
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	3	0.22
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	5	0.22
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	8	0.22
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	9	0.22
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	2	0.22
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	9	0.22
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	2	0.22
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	2	0.22
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	2	0.22
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	9	0.22
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	9	0.22
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	9	0.22
(1,3047)	1:112:A:GLN:HB3	1:113:A:GLY:H	2	0.22
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	7	0.22
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	1	0.22
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	4	0.22
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	9	0.22
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	2	0.22
(1,2732)	1:96:A:LYS:HD3	1:96:A:LYS:H	1	0.22
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	3	0.22
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	8	0.22
(1,2605)	1:90:A:THR:H	1:92:A:THR:H	4	0.22
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	6	0.22
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	2	0.22
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	1	0.22
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	1	0.22
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	3	0.22
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	3	0.22
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	1	0.22
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	3	0.22
(1,2437)	1:83:A:SER:HB3	1:83:A:SER:H	4	0.22
(1,2437)	1:83:A:SER:HB3	1:83:A:SER:H	5	0.22
(1,2437)	1:83:A:SER:HB3	1:83:A:SER:H	9	0.22
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	5	0.22
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	9	0.22
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	10	0.22
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	3	0.22
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	4	0.22
(1,2141)	1:65:A:ILE:HG12	1:65:A:ILE:H	1	0.22
(1,2138)	1:64:A:ARG:HB3	1:65:A:ILE:H	8	0.22
(1,2095)	1:58:A:VAL:HG11	1:58:A:VAL:H	3	0.22
(1,2095)	1:58:A:VAL:HG12	1:58:A:VAL:H	3	0.22
(1,2095)	1:58:A:VAL:HG13	1:58:A:VAL:H	3	0.22
(1,2095)	1:58:A:VAL:HG11	1:58:A:VAL:H	8	0.22
(1,2095)	1:58:A:VAL:HG12	1:58:A:VAL:H	8	0.22
(1,2095)	1:58:A:VAL:HG13	1:58:A:VAL:H	8	0.22
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	4	0.22
(1,2028)	1:51:A:ASN:H	1:53:A:LEU:H	8	0.22
(1,1969)	1:48:A:GLU:HG2	1:48:A:GLU:H	2	0.22
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	1	0.22
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	1	0.22
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	1	0.22
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	1	0.22
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	5	0.22
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	5	0.22
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	5	0.22
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	2	0.22
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	5	0.22
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	8	0.22
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	7	0.22
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	9	0.22
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	1	0.22
(1,1848)	1:42:A:TYR:HD1	1:43:A:LEU:H	10	0.22
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	1	0.22
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	2	0.22
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	6	0.22
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	3	0.22
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	7	0.22
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	8	0.22
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	2	0.22
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	1	0.22
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	1	0.22
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	1	0.22
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	3	0.22
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	9	0.22
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	5	0.22
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	7	0.22
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	9	0.22
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	7	0.22
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	9	0.22
(1,1578)	1:28:A:GLN:HG2	1:28:A:GLN:H	8	0.22
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	1	0.22
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	7	0.22
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	7	0.22
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	8	0.22
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	10	0.22
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	6	0.22
(1,1253)	1:11:A:VAL:H	1:13:A:GLU:H	8	0.22
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	4	0.22
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	8	0.22
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	8	0.22
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	9	0.22
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	9	0.22
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	4	0.22
(1,1141)	1:116:A:LEU:HD21	1:119:A:PHE:HE1	2	0.22
(1,1141)	1:116:A:LEU:HD21	1:119:A:PHE:HE2	2	0.22
(1,1141)	1:116:A:LEU:HD22	1:119:A:PHE:HE1	2	0.22
(1,1141)	1:116:A:LEU:HD22	1:119:A:PHE:HE2	2	0.22
(1,1141)	1:116:A:LEU:HD23	1:119:A:PHE:HE1	2	0.22
(1,1141)	1:116:A:LEU:HD23	1:119:A:PHE:HE2	2	0.22
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	1	0.22
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	1	0.22
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	1	0.22
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	3	0.22
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	3	0.22
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	3	0.22
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD3	4	0.22
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD2	10	0.22
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD3	10	0.22
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	4	0.22
(1,927)	1:93:A:GLU:HA	1:93:A:GLU:HG3	6	0.22
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	8	0.22
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	8	0.22
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	8	0.22
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	2	0.22
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	2	0.22
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	2	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	2	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	2	0.22
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	2	0.22
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	2	0.22
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	2	0.22
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	2	0.22
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	4	0.22
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	4	0.22
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	4	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	4	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	4	0.22
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	4	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	4	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	4	0.22
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	4	0.22
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	5	0.22
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	5	0.22
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	5	0.22
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	7	0.22
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	7	0.22
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	7	0.22
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	9	0.22
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	9	0.22
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	9	0.22
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	10	0.22
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	10	0.22
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	10	0.22
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	7	0.22
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	7	0.22
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	7	0.22
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	5	0.22
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	5	0.22
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	5	0.22
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	5	0.22
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	5	0.22
(1,722)	1:75:A:ALA:HB1	1:78:A:LYS:HG2	10	0.22
(1,722)	1:75:A:ALA:HB2	1:78:A:LYS:HG2	10	0.22
(1,722)	1:75:A:ALA:HB3	1:78:A:LYS:HG2	10	0.22
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	10	0.22
(1,700)	1:74:A:ARG:HA	1:74:A:ARG:HD2	9	0.22
(1,700)	1:74:A:ARG:HA	1:74:A:ARG:HD3	9	0.22
(1,640)	1:68:A:LEU:HD21	1:68:A:LEU:HA	1	0.22
(1,640)	1:68:A:LEU:HD22	1:68:A:LEU:HA	1	0.22
(1,640)	1:68:A:LEU:HD23	1:68:A:LEU:HA	1	0.22
(1,602)	1:60:A:ARG:HA	1:60:A:ARG:HD2	9	0.22
(1,602)	1:60:A:ARG:HA	1:60:A:ARG:HD3	9	0.22
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	4	0.22
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	10	0.22
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	4	0.22
(1,510)	1:47:A:LEU:HG	1:48:A:GLU:HB2	9	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	2	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	2	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	2	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	6	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	6	0.22
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	6	0.22
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	9	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	1	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	1	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	1	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	4	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	4	0.22
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	4	0.22
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	8	0.22
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	8	0.22
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	8	0.22
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	9	0.22
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	5	0.22
(1,319)	1:31:A:ALA:HA	1:100:A:VAL:HB	6	0.22
(1,313)	1:31:A:ALA:HA	1:33:A:MET:HB2	6	0.22
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	6	0.22
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	6	0.22
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	6	0.22
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	6	0.22
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	6	0.22
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	6	0.22
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	6	0.22
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	6	0.22
(1,186)	1:23:A:GLN:HG2	1:23:A:GLN:HA	10	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	2	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	2	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	4	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	4	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	5	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	5	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	6	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	6	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	9	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	9	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	10	0.22
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	10	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	6	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	6	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	6	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	6	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	6	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	6	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	6	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	6	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	6	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	9	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	9	0.22
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	9	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	9	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	9	0.22
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	9	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	9	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	9	0.22
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	9	0.22
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	1	0.22
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	1	0.22
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	1	0.22
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	9	0.22
(1,71)	1:11:A:VAL:HG11	1:35:A:LEU:HG	4	0.22
(1,71)	1:11:A:VAL:HG12	1:35:A:LEU:HG	4	0.22
(1,71)	1:11:A:VAL:HG13	1:35:A:LEU:HG	4	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	1	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	1	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	1	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	2	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	2	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	2	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	4	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	4	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	4	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	6	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	6	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	6	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	9	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	9	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	9	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	10	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	10	0.22
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	10	0.22
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	10	0.22
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	7	0.22
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	1	0.21
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	1	0.21
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	1	0.21
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	5	0.21
(1,3199)	1:80:A:PHE:HZ	1:109:A:LEU:HB2	10	0.21
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	9	0.21
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	3	0.21
(1,3077)	1:115:A:THR:HB	1:116:A:LEU:H	10	0.21
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	6	0.21
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	9	0.21
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	10	0.21
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	4	0.21
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	7	0.21
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	3	0.21
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	9	0.21
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	5	0.21
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	6	0.21
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	9	0.21
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	3	0.21
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	9	0.21
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	4	0.21
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	1	0.21
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	3	0.21
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	10	0.21
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	7	0.21
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	6	0.21
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	6	0.21
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	7	0.21
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	7	0.21
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	10	0.21
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	10	0.21
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	2	0.21
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	8	0.21
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	1	0.21
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	4	0.21
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	5	0.21
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	6	0.21
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	7	0.21
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	5	0.21
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	1	0.21
(1,2205)	1:72:A:GLU:HB2	1:74:A:ARG:H	4	0.21
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	2	0.21
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	9	0.21
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	1	0.21
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	1	0.21
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	1	0.21
(1,2041)	1:52:A:LEU:H	1:53:A:LEU:HA	1	0.21
(1,1955)	1:47:A:LEU:H	1:49:A:HIS:H	7	0.21
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	4	0.21
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	4	0.21
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	4	0.21
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	6	0.21
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	10	0.21
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	5	0.21
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	9	0.21
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	10	0.21
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	3	0.21
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	2	0.21
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	1	0.21
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	3	0.21
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	2	0.21
(1,1579)	1:28:A:GLN:HG3	1:28:A:GLN:H	4	0.21
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	10	0.21
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	1	0.21
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	7	0.21
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	4	0.21
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	1	0.21
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	1	0.21
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	5	0.21
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	6	0.21
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	6	0.21
(1,1063)	1:109:A:LEU:HD11	1:109:A:LEU:HB2	9	0.21
(1,1063)	1:109:A:LEU:HD12	1:109:A:LEU:HB2	9	0.21
(1,1063)	1:109:A:LEU:HD13	1:109:A:LEU:HB2	9	0.21
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	7	0.21
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	7	0.21
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	7	0.21
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	6	0.21
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	8	0.21
(1,996)	1:103:A:LEU:HA	1:105:A:VAL:HB	10	0.21
(1,962)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	7	0.21
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	3	0.21
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	3	0.21
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	3	0.21
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	1	0.21
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	1	0.21
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	1	0.21
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	2	0.21
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	2	0.21
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	2	0.21
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	4	0.21
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	4	0.21
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	4	0.21
(1,801)	1:81:A:LEU:HD21	1:81:A:LEU:HB3	8	0.21
(1,801)	1:81:A:LEU:HD22	1:81:A:LEU:HB3	8	0.21
(1,801)	1:81:A:LEU:HD23	1:81:A:LEU:HB3	8	0.21
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	3	0.21
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	3	0.21
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	3	0.21
(1,741)	1:77:A:LEU:HD11	1:80:A:PHE:HD2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:77:A:LEU:HD12	1:80:A:PHE:HD2	6	0.21
(1,741)	1:77:A:LEU:HD13	1:80:A:PHE:HD2	6	0.21
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	1	0.21
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	5	0.21
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	10	0.21
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	8	0.21
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG21	6	0.21
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG22	6	0.21
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG23	6	0.21
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD11	8	0.21
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD12	8	0.21
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD13	8	0.21
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD11	3	0.21
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD12	3	0.21
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD13	3	0.21
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	6	0.21
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	6	0.21
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	6	0.21
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	9	0.21
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	9	0.21
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	9	0.21
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	10	0.21
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	5	0.21
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	5	0.21
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	5	0.21
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	1	0.21
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB1	10	0.21
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB2	10	0.21
(1,372)	1:35:A:LEU:HD11	1:38:A:ALA:HB3	10	0.21
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB1	10	0.21
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB2	10	0.21
(1,372)	1:35:A:LEU:HD12	1:38:A:ALA:HB3	10	0.21
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB1	10	0.21
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB2	10	0.21
(1,372)	1:35:A:LEU:HD13	1:38:A:ALA:HB3	10	0.21
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	1	0.21
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	3	0.21
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	5	0.21
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	7	0.21
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	8	0.21
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	8	0.21
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	8	0.21
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	8	0.21
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	8	0.21
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	8	0.21
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	8	0.21
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	8	0.21
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	3	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	5	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	5	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	5	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	5	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	5	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	5	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	5	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	5	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	5	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	7	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	7	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	7	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	7	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	7	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	7	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	7	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	7	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	7	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	10	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	10	0.21
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	10	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	10	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	10	0.21
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	10	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	10	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	10	0.21
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	10	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	3	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	3	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	7	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	7	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD1	8	0.21
(1,141)	1:18:A:PHE:HA	1:18:A:PHE:HD2	8	0.21
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	7	0.21
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	7	0.21
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	7	0.21
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	7	0.21
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	7	0.21
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	7	0.21
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	7	0.21
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	7	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	3	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	3	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	3	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	6	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	6	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	6	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	7	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	7	0.21
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	7	0.21
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	2	0.21
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	5	0.21
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	5	0.21
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	5	0.21
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	7	0.21
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	1	0.21
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	7	0.2
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	6	0.2
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	6	0.2
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	6	0.2
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	6	0.2
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	10	0.2
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	4	0.2
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	6	0.2
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	1	0.2
(1,3028)	1:111:A:ARG:HG3	1:113:A:GLY:H	6	0.2
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	1	0.2
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	3	0.2
(1,2996)	1:110:A:LYS:HG3	1:110:A:LYS:H	5	0.2
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	1	0.2
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	5	0.2
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	6	0.2
(1,2954)	1:108:A:ALA:H	1:109:A:LEU:HA	6	0.2
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	6	0.2
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	2	0.2
(1,2732)	1:96:A:LYS:HD3	1:96:A:LYS:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	1	0.2
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	6	0.2
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	9	0.2
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG21	9	0.2
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG22	9	0.2
(1,2561)	1:88:A:SER:H	1:89:A:VAL:HG23	9	0.2
(1,2542)	1:87:A:ASP:HB3	1:88:A:SER:H	8	0.2
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	10	0.2
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	2	0.2
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	5	0.2
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	6	0.2
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	2	0.2
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	9	0.2
(1,2423)	1:82:A:GLU:HB3	1:83:A:SER:H	10	0.2
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	2	0.2
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	9	0.2
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	3	0.2
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	5	0.2
(1,2139)	1:64:A:ARG:H	1:65:A:ILE:H	8	0.2
(1,2131)	1:63:A:LYS:H	1:64:A:ARG:HG3	2	0.2
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	2	0.2
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	2	0.2
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	2	0.2
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	5	0.2
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	5	0.2
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	5	0.2
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	10	0.2
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	10	0.2
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	10	0.2
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	3	0.2
(1,2080)	1:56:A:HIS:HA	1:58:A:VAL:H	9	0.2
(1,2041)	1:52:A:LEU:H	1:53:A:LEU:HA	6	0.2
(1,2041)	1:52:A:LEU:H	1:53:A:LEU:HA	10	0.2
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	3	0.2
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	3	0.2
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	3	0.2
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	7	0.2
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	7	0.2
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	7	0.2
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	9	0.2
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	9	0.2
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	1	0.2
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	3	0.2
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	4	0.2
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	2	0.2
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	9	0.2
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	8	0.2
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	6	0.2
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	7	0.2
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	2	0.2
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	7	0.2
(1,1648)	1:31:A:ALA:HA	1:101:A:THR:H	5	0.2
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	9	0.2
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	2	0.2
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	4	0.2
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	6	0.2
(1,1586)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	10	0.2
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	6	0.2
(1,1530)	1:26:A:ARG:HD2	1:27:A:TRP:H	10	0.2
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	4	0.2
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	5	0.2
(1,1489)	1:24:A:ASP:HB3	1:24:A:ASP:H	2	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	1	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	1	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	1	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	6	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	6	0.2
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	6	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	2	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	2	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	2	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	3	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	3	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	3	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	7	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	7	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	7	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	8	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	8	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	8	0.2
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	10	0.2
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	10	0.2
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	1	0.2
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	8	0.2
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	10	0.2
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	7	0.2
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	7	0.2
(1,1168)	1:2:A:ILE:HG12	1:4:A:LYS:H	5	0.2
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	9	0.2
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	2	0.2
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	3	0.2
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	6	0.2
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	6	0.2
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	6	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	4	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	4	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	4	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	4	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	4	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	4	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	4	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	4	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	4	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	5	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	5	0.2
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	5	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	5	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	5	0.2
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	5	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	5	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	5	0.2
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	5	0.2
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	2	0.2
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	2	0.2
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	2	0.2
(1,950)	1:96:A:LYS:HD3	1:96:A:LYS:HB2	4	0.2
(1,950)	1:96:A:LYS:HD3	1:96:A:LYS:HB2	8	0.2
(1,950)	1:96:A:LYS:HD3	1:96:A:LYS:HB2	10	0.2
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	10	0.2
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	10	0.2
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	10	0.2
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	1	0.2
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	1	0.2
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	1	0.2
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	1	0.2
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	1	0.2
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	1	0.2
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	1	0.2
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	1	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	2	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	2	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	2	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	2	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	2	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	2	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	2	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	2	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	2	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	3	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	3	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	3	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	3	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	3	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	3	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	3	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	3	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	3	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	7	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	7	0.2
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	7	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	7	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	7	0.2
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	7	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	7	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	7	0.2
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	7	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	5	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	5	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	5	0.2
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	5	0.2
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	5	0.2
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	5	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	10	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	10	0.2
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	10	0.2
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	10	0.2
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	10	0.2
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	3	0.2
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	3	0.2
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	3	0.2
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	3	0.2
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	3	0.2
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	3	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	3	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	4	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	6	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	8	0.2
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	9	0.2
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	9	0.2
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	2	0.2
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	2	0.2
(1,629)	1:65:A:ILE:HA	1:67:A:GLY:HA3	1	0.2
(1,624)	1:65:A:ILE:HA	1:65:A:ILE:HG12	8	0.2
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	10	0.2
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	10	0.2
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	10	0.2
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	10	0.2
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	10	0.2
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	10	0.2
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD2	9	0.2
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD3	9	0.2
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD2	10	0.2
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD3	10	0.2
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	1	0.2
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	1	0.2
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	3	0.2
(1,569)	1:57:A:LEU:HA	1:57:A:LEU:HG	3	0.2
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	3	0.2
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	3	0.2
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	3	0.2
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	7	0.2
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	4	0.2
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	7	0.2
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	7	0.2
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	7	0.2
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	9	0.2
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	9	0.2
(1,398)	1:40:A:GLU:HG3	1:41:A:ALA:HA	5	0.2
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	3	0.2
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	4	0.2
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	5	0.2
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	6	0.2
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	8	0.2
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	2	0.2
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	2	0.2
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	2	0.2
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	7	0.2
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	7	0.2
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	7	0.2
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	1	0.2
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	1	0.2
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	1	0.2
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	1	0.2
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	1	0.2
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	1	0.2
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	1	0.2
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	1	0.2
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	1	0.2
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD11	2	0.2
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD12	2	0.2
(1,134)	1:15:A:THR:HG21	1:85:A:ILE:HD13	2	0.2
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD11	2	0.2
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD12	2	0.2
(1,134)	1:15:A:THR:HG22	1:85:A:ILE:HD13	2	0.2
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD11	2	0.2
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD12	2	0.2
(1,134)	1:15:A:THR:HG23	1:85:A:ILE:HD13	2	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	2	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	2	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	2	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	5	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	5	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	5	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	10	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	10	0.2
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	10	0.2
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:11:A:VAL:HB	1:35:A:LEU:HA	9	0.2
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	4	0.2
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	5	0.2
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	5	0.2
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	10	0.19
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	3	0.19
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	7	0.19
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	6	0.19
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	7	0.19
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	8	0.19
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	7	0.19
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	10	0.19
(1,3095)	1:117:A:TYR:HB3	1:117:A:TYR:H	6	0.19
(1,3089)	1:116:A:LEU:HG	1:117:A:TYR:H	1	0.19
(1,3073)	1:115:A:THR:HG21	1:115:A:THR:H	5	0.19
(1,3073)	1:115:A:THR:HG22	1:115:A:THR:H	5	0.19
(1,3073)	1:115:A:THR:HG23	1:115:A:THR:H	5	0.19
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	7	0.19
(1,3064)	1:114:A:ARG:H	1:115:A:THR:HA	3	0.19
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	4	0.19
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	7	0.19
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	2	0.19
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	6	0.19
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	1	0.19
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	4	0.19
(1,2740)	1:96:A:LYS:HE2	1:98:A:LYS:H	1	0.19
(1,2740)	1:96:A:LYS:HE3	1:98:A:LYS:H	1	0.19
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	6	0.19
(1,2703)	1:93:A:GLU:HA	1:98:A:LYS:H	10	0.19
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	1	0.19
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	3	0.19
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	5	0.19
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	6	0.19
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	2	0.19
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	10	0.19
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	6	0.19
(1,2564)	1:88:A:SER:H	1:90:A:THR:HA	9	0.19
(1,2563)	1:88:A:SER:H	1:90:A:THR:HB	9	0.19
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	9	0.19
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	4	0.19
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	9	0.19
(1,2453)	1:83:A:SER:HB2	1:86:A:ARG:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2453)	1:83:A:SER:HB3	1:86:A:ARG:H	8	0.19
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	7	0.19
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	2	0.19
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	7	0.19
(1,2427)	1:82:A:GLU:H	1:84:A:VAL:HA	8	0.19
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	2	0.19
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	9	0.19
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	1	0.19
(1,2243)	1:74:A:ARG:HB3	1:75:A:ALA:H	6	0.19
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	3	0.19
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	6	0.19
(1,2173)	1:69:A:ILE:HG12	1:69:A:ILE:H	8	0.19
(1,2127)	1:62:A:SER:HB2	1:64:A:ARG:H	4	0.19
(1,2095)	1:58:A:VAL:HG11	1:58:A:VAL:H	7	0.19
(1,2095)	1:58:A:VAL:HG12	1:58:A:VAL:H	7	0.19
(1,2095)	1:58:A:VAL:HG13	1:58:A:VAL:H	7	0.19
(1,2094)	1:58:A:VAL:HG21	1:58:A:VAL:H	9	0.19
(1,2094)	1:58:A:VAL:HG22	1:58:A:VAL:H	9	0.19
(1,2094)	1:58:A:VAL:HG23	1:58:A:VAL:H	9	0.19
(1,2059)	1:54:A:ALA:HA	1:56:A:HIS:H	9	0.19
(1,2007)	1:51:A:ASN:HB3	1:51:A:ASN:HD22	7	0.19
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	2	0.19
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	2	0.19
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	2	0.19
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	6	0.19
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	6	0.19
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	6	0.19
(1,1891)	1:44:A:VAL:HG21	1:45:A:GLY:H	10	0.19
(1,1891)	1:44:A:VAL:HG22	1:45:A:GLY:H	10	0.19
(1,1891)	1:44:A:VAL:HG23	1:45:A:GLY:H	10	0.19
(1,1884)	1:43:A:LEU:HB2	1:46:A:LEU:H	7	0.19
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	3	0.19
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	4	0.19
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	5	0.19
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	7	0.19
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	3	0.19
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	2	0.19
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	1	0.19
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	4	0.19
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	10	0.19
(1,1651)	1:31:A:ALA:HB1	1:102:A:SER:H	4	0.19
(1,1651)	1:31:A:ALA:HB2	1:102:A:SER:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:31:A:ALA:HB3	1:102:A:SER:H	4	0.19
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	1	0.19
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	5	0.19
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	8	0.19
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	8	0.19
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	6	0.19
(1,1585)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	8	0.19
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	2	0.19
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	3	0.19
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	8	0.19
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	8	0.19
(1,1517)	1:25:A:LEU:HB3	1:99:A:THR:H	8	0.19
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	5	0.19
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	9	0.19
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	4	0.19
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	4	0.19
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	4	0.19
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	8	0.19
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	8	0.19
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	8	0.19
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	4	0.19
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	4	0.19
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	4	0.19
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	5	0.19
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	5	0.19
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	5	0.19
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	6	0.19
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	6	0.19
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	6	0.19
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	9	0.19
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	9	0.19
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	9	0.19
(1,1373)	1:17:A:GLU:H	1:18:A:PHE:HA	4	0.19
(1,1304)	1:13:A:GLU:H	1:15:A:THR:HB	4	0.19
(1,1304)	1:13:A:GLU:H	1:15:A:THR:HB	8	0.19
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	6	0.19
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	3	0.19
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	3	0.19
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	2	0.19
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	2	0.19
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	9	0.19
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	4	0.19
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	4	0.19
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	4	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	2	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	2	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	2	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	2	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	2	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	2	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	2	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	2	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	2	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	3	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	3	0.19
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	3	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	3	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	3	0.19
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	3	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	3	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	3	0.19
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	3	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	6	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	6	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	6	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	6	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	6	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	6	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	8	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	8	0.19
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	8	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	8	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	8	0.19
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	8	0.19
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	6	0.19
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	6	0.19
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	6	0.19
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD11	6	0.19
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD12	6	0.19
(1,810)	1:81:A:LEU:HD11	1:85:A:ILE:HD13	6	0.19
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD11	6	0.19
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD12	6	0.19
(1,810)	1:81:A:LEU:HD12	1:85:A:ILE:HD13	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD11	6	0.19
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD12	6	0.19
(1,810)	1:81:A:LEU:HD13	1:85:A:ILE:HD13	6	0.19
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	7	0.19
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	7	0.19
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	7	0.19
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	7	0.19
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	7	0.19
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	7	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	1	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	3	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	4	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	5	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	6	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	9	0.19
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	10	0.19
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	7	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	1	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	3	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	5	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	6	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	8	0.19
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	9	0.19
(1,706)	1:74:A:ARG:HD3	1:74:A:ARG:HB3	9	0.19
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	6	0.19
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	6	0.19
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD11	3	0.19
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD12	3	0.19
(1,626)	1:65:A:ILE:HA	1:65:A:ILE:HD13	3	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	2	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	3	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	4	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	5	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	6	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	7	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	9	0.19
(1,593)	1:59:A:PRO:HD2	1:59:A:PRO:HA	10	0.19
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	2	0.19
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	5	0.19
(1,591)	1:59:A:PRO:HD3	1:59:A:PRO:HA	7	0.19
(1,590)	1:58:A:VAL:HG21	1:60:A:ARG:HG2	8	0.19
(1,590)	1:58:A:VAL:HG21	1:60:A:ARG:HG3	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:58:A:VAL:HG22	1:60:A:ARG:HG2	8	0.19
(1,590)	1:58:A:VAL:HG22	1:60:A:ARG:HG3	8	0.19
(1,590)	1:58:A:VAL:HG23	1:60:A:ARG:HG2	8	0.19
(1,590)	1:58:A:VAL:HG23	1:60:A:ARG:HG3	8	0.19
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	7	0.19
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	7	0.19
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	7	0.19
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	10	0.19
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	10	0.19
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	10	0.19
(1,525)	1:51:A:ASN:HB3	1:54:A:ALA:HB1	9	0.19
(1,525)	1:51:A:ASN:HB3	1:54:A:ALA:HB2	9	0.19
(1,525)	1:51:A:ASN:HB3	1:54:A:ALA:HB3	9	0.19
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG21	7	0.19
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG22	7	0.19
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG23	7	0.19
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	1	0.19
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	1	0.19
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	1	0.19
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	10	0.19
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD11	9	0.19
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD12	9	0.19
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD13	9	0.19
(1,398)	1:40:A:GLU:HG3	1:41:A:ALA:HA	6	0.19
(1,398)	1:40:A:GLU:HG3	1:41:A:ALA:HA	7	0.19
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	2	0.19
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	2	0.19
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	6	0.19
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	3	0.19
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	3	0.19
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	3	0.19
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	5	0.19
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	5	0.19
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	5	0.19
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	10	0.19
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	10	0.19
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	10	0.19
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	6	0.19
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	1	0.19
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	1	0.19
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	1	0.19
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	1	0.19
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	1	0.19
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	1	0.19
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	1	0.19
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	1	0.19
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	6	0.19
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	10	0.19
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD11	2	0.19
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD12	2	0.19
(1,189)	1:23:A:GLN:HB3	1:25:A:LEU:HD13	2	0.19
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	2	0.19
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	2	0.19
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	2	0.19
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	2	0.19
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	2	0.19
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	2	0.19
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	2	0.19
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	2	0.19
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	2	0.19
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	5	0.19
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	8	0.19
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	9	0.19
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	10	0.19
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	1	0.19
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	1	0.19
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	6	0.19
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	6	0.19
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	6	0.19
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	3	0.19
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	6	0.19
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	2	0.18
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	6	0.18
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	8	0.18
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	9	0.18
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	3	0.18
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	3	0.18
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	3	0.18
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	2	0.18
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	1	0.18
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	1	0.18
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	3	0.18
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	7	0.18
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	9	0.18
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	2	0.18
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	6	0.18
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	6	0.18
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	6	0.18
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	4	0.18
(1,3070)	1:114:A:ARG:HB2	1:115:A:THR:H	9	0.18
(1,3067)	1:114:A:ARG:HB3	1:115:A:THR:H	10	0.18
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	2	0.18
(1,3029)	1:111:A:ARG:HG2	1:113:A:GLY:H	6	0.18
(1,3024)	1:111:A:ARG:HG2	1:112:A:GLN:H	6	0.18
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	2	0.18
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	8	0.18
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	10	0.18
(1,2853)	1:103:A:LEU:HG	1:105:A:VAL:H	5	0.18
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	2	0.18
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	5	0.18
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	9	0.18
(1,2757)	1:97:A:ARG:HB3	1:98:A:LYS:H	2	0.18
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	3	0.18
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	9	0.18
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	5	0.18
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	7	0.18
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	8	0.18
(1,2732)	1:96:A:LYS:HD3	1:96:A:LYS:H	4	0.18
(1,2732)	1:96:A:LYS:HD3	1:96:A:LYS:H	10	0.18
(1,2712)	1:94:A:HIS:H	1:96:A:LYS:HG3	10	0.18
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	3	0.18
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	2	0.18
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	8	0.18
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	8	0.18
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	1	0.18
(1,2542)	1:87:A:ASP:HB3	1:88:A:SER:H	9	0.18
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	2	0.18
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	6	0.18
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	3	0.18
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	6	0.18
(1,2452)	1:83:A:SER:HA	1:86:A:ARG:H	10	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	1	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	3	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	5	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	6	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	8	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	9	0.18
(1,2441)	1:83:A:SER:H	1:84:A:VAL:HA	10	0.18
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	4	0.18
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	7	0.18
(1,2297)	1:77:A:LEU:H	1:78:A:LYS:HB3	8	0.18
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	1	0.18
(1,2255)	1:74:A:ARG:H	1:77:A:LEU:HG	9	0.18
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	4	0.18
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	6	0.18
(1,2082)	1:57:A:LEU:HD21	1:57:A:LEU:H	7	0.18
(1,2082)	1:57:A:LEU:HD22	1:57:A:LEU:H	7	0.18
(1,2082)	1:57:A:LEU:HD23	1:57:A:LEU:H	7	0.18
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	8	0.18
(1,2011)	1:51:A:ASN:HA	1:51:A:ASN:HD21	5	0.18
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG21	5	0.18
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG22	5	0.18
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG23	5	0.18
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	7	0.18
(1,1784)	1:38:A:ALA:H	1:40:A:GLU:HG3	10	0.18
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	5	0.18
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	10	0.18
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	5	0.18
(1,1650)	1:31:A:ALA:H	1:102:A:SER:HA	10	0.18
(1,1639)	1:31:A:ALA:H	1:33:A:MET:H	6	0.18
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	3	0.18
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	1	0.18
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	2	0.18
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	10	0.18
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	3	0.18
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	3	0.18
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	3	0.18
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	10	0.18
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	2	0.18
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	5	0.18
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	7	0.18
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	9	0.18
(1,1250)	1:11:A:VAL:HB	1:12:A:LYS:H	8	0.18
(1,1250)	1:11:A:VAL:HB	1:12:A:LYS:H	9	0.18
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:10:A:LEU:HD21	1:10:A:LEU:H	8	0.18
(1,1225)	1:10:A:LEU:HD22	1:10:A:LEU:H	8	0.18
(1,1225)	1:10:A:LEU:HD23	1:10:A:LEU:H	8	0.18
(1,1152)	1:117:A:TYR:HB2	1:119:A:PHE:HB3	8	0.18
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	6	0.18
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	7	0.18
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	3	0.18
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	3	0.18
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	3	0.18
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	4	0.18
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	4	0.18
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	4	0.18
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	8	0.18
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	8	0.18
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	8	0.18
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	5	0.18
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	5	0.18
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	5	0.18
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	10	0.18
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	10	0.18
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	10	0.18
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	10	0.18
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	10	0.18
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	10	0.18
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	10	0.18
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	10	0.18
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	10	0.18
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	10	0.18
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	10	0.18
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	10	0.18
(1,962)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	5	0.18
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	3	0.18
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	3	0.18
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	3	0.18
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	7	0.18
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	7	0.18
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	1	0.18
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	1	0.18
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	1	0.18
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	3	0.18
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	3	0.18
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	6	0.18
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	6	0.18
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	6	0.18
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	6	0.18
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	6	0.18
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	6	0.18
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	6	0.18
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	6	0.18
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	6	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	8	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	8	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	8	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	10	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	10	0.18
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	10	0.18
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	8	0.18
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	8	0.18
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	8	0.18
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	8	0.18
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	8	0.18
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	8	0.18
(1,752)	1:77:A:LEU:HB2	1:81:A:LEU:HD11	1	0.18
(1,752)	1:77:A:LEU:HB2	1:81:A:LEU:HD12	1	0.18
(1,752)	1:77:A:LEU:HB2	1:81:A:LEU:HD13	1	0.18
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	2	0.18
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	7	0.18
(1,748)	1:77:A:LEU:HA	1:80:A:PHE:HB3	8	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	2	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	2	0.18
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	2	0.18
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	2	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	2	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	2	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	7	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	7	0.18
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	7	0.18
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	7	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	7	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	7	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	8	0.18
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	8	0.18
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	8	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	8	0.18
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	8	0.18
(1,721)	1:75:A:ALA:HA	1:78:A:LYS:HB3	2	0.18
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	7	0.18
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	10	0.18
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD11	5	0.18
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD12	5	0.18
(1,621)	1:64:A:ARG:HB2	1:65:A:ILE:HD13	5	0.18
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD11	5	0.18
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD12	5	0.18
(1,621)	1:64:A:ARG:HB3	1:65:A:ILE:HD13	5	0.18
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	3	0.18
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	3	0.18
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	3	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	5	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	5	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	5	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	7	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	7	0.18
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	7	0.18
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	6	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	2	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	2	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	2	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	3	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	3	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	3	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	6	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	6	0.18
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	6	0.18
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	9	0.18
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	9	0.18
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	9	0.18
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	9	0.18
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	9	0.18
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	9	0.18
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	9	0.18
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	9	0.18
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	9	0.18
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	8	0.18
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	8	0.18
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	7	0.18
(1,382)	1:38:A:ALA:HA	1:39:A:SER:HA	10	0.18
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	7	0.18
(1,242)	1:26:A:ARG:HB2	1:99:A:THR:HG21	4	0.18
(1,242)	1:26:A:ARG:HB2	1:99:A:THR:HG22	4	0.18
(1,242)	1:26:A:ARG:HB2	1:99:A:THR:HG23	4	0.18
(1,242)	1:26:A:ARG:HB3	1:99:A:THR:HG21	4	0.18
(1,242)	1:26:A:ARG:HB3	1:99:A:THR:HG22	4	0.18
(1,242)	1:26:A:ARG:HB3	1:99:A:THR:HG23	4	0.18
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	2	0.18
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	9	0.18
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	1	0.18
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	3	0.18
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	3	0.18
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	3	0.18
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	3	0.18
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	3	0.18
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	3	0.18
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	3	0.18
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	3	0.18
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	3	0.18
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	1	0.18
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	1	0.18
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	1	0.18
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	1	0.18
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	1	0.18
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	1	0.18
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	1	0.18
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	1	0.18
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	1	0.18
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	1	0.18
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	1	0.18
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	1	0.18
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	9	0.18
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	9	0.18
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	9	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	1	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	2	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	3	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	4	0.18
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	8	0.18
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	8	0.18
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	8	0.18
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	8	0.18
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	8	0.18
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	8	0.18
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	7	0.18
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	10	0.18
(1,71)	1:11:A:VAL:HG11	1:35:A:LEU:HG	1	0.18
(1,71)	1:11:A:VAL:HG12	1:35:A:LEU:HG	1	0.18
(1,71)	1:11:A:VAL:HG13	1:35:A:LEU:HG	1	0.18
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	10	0.18
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	3	0.17
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	5	0.17
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	10	0.17
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	7	0.17
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	7	0.17
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	7	0.17
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	2	0.17
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	5	0.17
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	10	0.17
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	6	0.17
(1,3076)	1:115:A:THR:H	1:116:A:LEU:HA	7	0.17
(1,3036)	1:112:A:GLN:HB2	1:112:A:GLN:HE21	7	0.17
(1,3010)	1:110:A:LYS:HB2	1:116:A:LEU:H	6	0.17
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	3	0.17
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	9	0.17
(1,2950)	1:107:A:TYR:H	1:110:A:LYS:HB2	6	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	1	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	3	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	4	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	5	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	7	0.17
(1,2941)	1:107:A:TYR:H	1:108:A:ALA:HA	9	0.17
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	7	0.17
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	5	0.17
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	4	0.17
(1,2712)	1:94:A:HIS:H	1:96:A:LYS:HG3	4	0.17
(1,2703)	1:93:A:GLU:HA	1:98:A:LYS:H	8	0.17
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	10	0.17
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	1	0.17
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	2	0.17
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	7	0.17
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	5	0.17
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	1	0.17
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	3	0.17
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	4	0.17
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	7	0.17
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	3	0.17
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	5	0.17
(1,2173)	1:69:A:ILE:HG12	1:69:A:ILE:H	5	0.17
(1,2156)	1:66:A:SER:HB2	1:68:A:LEU:H	10	0.17
(1,2143)	1:65:A:ILE:HB	1:65:A:ILE:H	8	0.17
(1,2141)	1:65:A:ILE:HG12	1:65:A:ILE:H	3	0.17
(1,2134)	1:64:A:ARG:HB2	1:64:A:ARG:H	4	0.17
(1,2090)	1:57:A:LEU:HG	1:58:A:VAL:H	6	0.17
(1,2071)	1:55:A:LEU:H	1:57:A:LEU:H	3	0.17
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	10	0.17
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	6	0.17
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	3	0.17
(1,1775)	1:37:A:GLU:H	1:40:A:GLU:HG3	10	0.17
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	1	0.17
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	3	0.17
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	10	0.17
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	7	0.17
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	10	0.17
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	3	0.17
(1,1611)	1:30:A:MET:HG2	1:30:A:MET:H	1	0.17
(1,1611)	1:30:A:MET:HG2	1:30:A:MET:H	5	0.17
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	7	0.17
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	5	0.17
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	5	0.17
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	5	0.17
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	5	0.17
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	8	0.17
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	8	0.17
(1,1441)	1:21:A:LYS:HB2	1:24:A:ASP:H	2	0.17
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	1	0.17
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	6	0.17
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	7	0.17
(1,1408)	1:19:A:THR:HG21	1:20:A:THR:H	1	0.17
(1,1408)	1:19:A:THR:HG22	1:20:A:THR:H	1	0.17
(1,1408)	1:19:A:THR:HG23	1:20:A:THR:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	10	0.17
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	2	0.17
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	8	0.17
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	8	0.17
(1,1133)	1:116:A:LEU:HA	1:116:A:LEU:HG	2	0.17
(1,1116)	1:114:A:ARG:HB3	1:114:A:ARG:HD3	3	0.17
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	1	0.17
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	4	0.17
(1,1105)	1:111:A:ARG:HA	1:112:A:GLN:HB2	2	0.17
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	1	0.17
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	8	0.17
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	2	0.17
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	2	0.17
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	2	0.17
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	5	0.17
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	5	0.17
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	5	0.17
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	5	0.17
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	7	0.17
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	8	0.17
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	10	0.17
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	6	0.17
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	10	0.17
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	5	0.17
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	5	0.17
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	6	0.17
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	6	0.17
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	9	0.17
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	9	0.17
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG21	8	0.17
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG22	8	0.17
(1,889)	1:89:A:VAL:HG11	1:100:A:VAL:HG23	8	0.17
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG21	8	0.17
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG22	8	0.17
(1,889)	1:89:A:VAL:HG12	1:100:A:VAL:HG23	8	0.17
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG21	8	0.17
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG22	8	0.17
(1,889)	1:89:A:VAL:HG13	1:100:A:VAL:HG23	8	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	2	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	2	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	2	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	3	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	3	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	6	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	6	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	6	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	7	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	7	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	7	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	10	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	10	0.17
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	10	0.17
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	6	0.17
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	6	0.17
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	6	0.17
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD11	8	0.17
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD12	8	0.17
(1,811)	1:81:A:LEU:HB2	1:85:A:ILE:HD13	8	0.17
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	1	0.17
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	1	0.17
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	1	0.17
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	1	0.17
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	1	0.17
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	1	0.17
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	4	0.17
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	4	0.17
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	4	0.17
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	4	0.17
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	4	0.17
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	4	0.17
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG2	9	0.17
(1,732)	1:76:A:VAL:HG21	1:78:A:LYS:HG3	9	0.17
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG2	9	0.17
(1,732)	1:76:A:VAL:HG22	1:78:A:LYS:HG3	9	0.17
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG2	9	0.17
(1,732)	1:76:A:VAL:HG23	1:78:A:LYS:HG3	9	0.17
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	4	0.17
(1,624)	1:65:A:ILE:HA	1:65:A:ILE:HG12	2	0.17
(1,537)	1:53:A:LEU:HG	1:53:A:LEU:HA	6	0.17
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	1	0.17
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	1	0.17
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	1	0.17
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	8	0.17
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	8	0.17
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	3	0.17
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	4	0.17
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	1	0.17
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	5	0.17
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	7	0.17
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	8	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	5	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	5	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	5	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	9	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD22	9	0.17
(1,434)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	9	0.17
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	1	0.17
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	4	0.17
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	6	0.17
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	6	0.17
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	6	0.17
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	6	0.17
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	6	0.17
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	6	0.17
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	6	0.17
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	6	0.17
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	6	0.17
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	5	0.17
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	7	0.17
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	9	0.17
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	9	0.17
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	9	0.17
(1,236)	1:26:A:ARG:HB2	1:99:A:THR:HA	4	0.17
(1,236)	1:26:A:ARG:HB3	1:99:A:THR:HA	4	0.17
(1,229)	1:26:A:ARG:HA	1:26:A:ARG:HD3	8	0.17
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	3	0.17
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	3	0.17
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	3	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	7	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	7	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	7	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	7	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	7	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	7	0.17
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	7	0.17
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	7	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	8	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	8	0.17
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	8	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	8	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	8	0.17
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	8	0.17
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	8	0.17
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	8	0.17
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	8	0.17
(1,99)	1:13:A:GLU:HA	1:13:A:GLU:HG3	7	0.17
(1,70)	1:11:A:VAL:HB	1:35:A:LEU:HA	8	0.17
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	3	0.17
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	2	0.17
(1,40)	1:9:A:ARG:HD3	1:9:A:ARG:HB2	2	0.17
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	2	0.17
(2,26)	1:29:A:SER:O	1:33:A:MET:N	6	0.16
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	1	0.16
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	4	0.16
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	7	0.16
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD21	7	0.16
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD22	7	0.16
(1,3202)	1:80:A:PHE:HE1	1:109:A:LEU:HD23	7	0.16
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	8	0.16
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	4	0.16
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	2	0.16
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	9	0.16
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	9	0.16
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	10	0.16
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	7	0.16
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	4	0.16
(1,3151)	1:27:A:TRP:HB3	1:27:A:TRP:HD1	8	0.16
(1,3130)	1:15:A:THR:HA	1:18:A:PHE:HZ	1	0.16
(1,3102)	1:117:A:TYR:HA	1:118:A:GLY:H	3	0.16
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	7	0.16
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	7	0.16
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	7	0.16
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	3	0.16
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	10	0.16
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	7	0.16
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	10	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	5	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	5	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	5	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	8	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	8	0.16
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	8	0.16
(1,2853)	1:103:A:LEU:HG	1:105:A:VAL:H	2	0.16
(1,2853)	1:103:A:LEU:HG	1:105:A:VAL:H	10	0.16
(1,2848)	1:103:A:LEU:HB2	1:104:A:ASP:H	8	0.16
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	10	0.16
(1,2813)	1:101:A:THR:H	1:104:A:ASP:HB3	5	0.16
(1,2765)	1:98:A:LYS:HG3	1:98:A:LYS:H	7	0.16
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	8	0.16
(1,2712)	1:94:A:HIS:H	1:96:A:LYS:HG3	1	0.16
(1,2712)	1:94:A:HIS:H	1:96:A:LYS:HG3	8	0.16
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	1	0.16
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	2	0.16
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	4	0.16
(1,2701)	1:93:A:GLU:HB2	1:97:A:ARG:H	9	0.16
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	10	0.16
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	3	0.16
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	8	0.16
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	10	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	1	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	2	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	6	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	8	0.16
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	10	0.16
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	4	0.16
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	5	0.16
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	8	0.16
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	9	0.16
(1,2278)	1:76:A:VAL:H	1:77:A:LEU:HG	8	0.16
(1,2273)	1:76:A:VAL:HB	1:77:A:LEU:H	9	0.16
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	9	0.16
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	9	0.16
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	9	0.16
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	10	0.16
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	2	0.16
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	1	0.16
(1,2138)	1:64:A:ARG:HB3	1:65:A:ILE:H	1	0.16
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	1	0.16
(1,2004)	1:51:A:ASN:HB3	1:51:A:ASN:H	4	0.16
(1,2000)	1:50:A:THR:HB	1:51:A:ASN:H	6	0.16
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG21	7	0.16
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG22	7	0.16
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG23	7	0.16
(1,1876)	1:43:A:LEU:HB3	1:45:A:GLY:H	8	0.16
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	9	0.16
(1,1830)	1:41:A:ALA:HA	1:43:A:LEU:H	10	0.16
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	1	0.16
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	2	0.16
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	4	0.16
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	9	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	1	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	1	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	2	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	2	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	3	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	3	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	4	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	4	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	5	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	5	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	8	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	8	0.16
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	9	0.16
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	9	0.16
(1,1727)	1:35:A:LEU:H	1:36:A:GLN:HA	6	0.16
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	7	0.16
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	8	0.16
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	9	0.16
(1,1691)	1:33:A:MET:H	1:35:A:LEU:HB2	5	0.16
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	3	0.16
(1,1672)	1:32:A:ILE:H	1:35:A:LEU:H	5	0.16
(1,1669)	1:32:A:ILE:HB	1:35:A:LEU:H	6	0.16
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	1	0.16
(1,1611)	1:30:A:MET:HG2	1:30:A:MET:H	7	0.16
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	2	0.16
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	9	0.16
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	7	0.16
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	1	0.16
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	6	0.16
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	8	0.16
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	7	0.16
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	7	0.16
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	7	0.16
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	7	0.16
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	7	0.16
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	7	0.16
(1,1482)	1:23:A:GLN:HA	1:25:A:LEU:H	2	0.16
(1,1477)	1:23:A:GLN:HB2	1:24:A:ASP:H	10	0.16
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	4	0.16
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	9	0.16
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	3	0.16
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	8	0.16
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	4	0.16
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	1	0.16
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	1	0.16
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	1	0.16
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	2	0.16
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	2	0.16
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	2	0.16
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	6	0.16
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	6	0.16
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	6	0.16
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	7	0.16
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	7	0.16
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	7	0.16
(1,1239)	1:10:A:LEU:HA	1:13:A:GLU:H	7	0.16
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	3	0.16
(1,1184)	1:7:A:PHE:HD1	1:10:A:LEU:H	5	0.16
(1,1184)	1:7:A:PHE:HD2	1:10:A:LEU:H	5	0.16
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	10	0.16
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD1	6	0.16
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD2	6	0.16
(1,1119)	1:114:A:ARG:HA	1:114:A:ARG:HG3	9	0.16
(1,1116)	1:114:A:ARG:HB3	1:114:A:ARG:HD3	5	0.16
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	8	0.16
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	10	0.16
(1,1111)	1:113:A:GLY:HA3	1:114:A:ARG:HG3	9	0.16
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	10	0.16
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	9	0.16
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	9	0.16
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	9	0.16
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	2	0.16
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	3	0.16
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	9	0.16
(1,964)	1:98:A:LYS:HD2	1:98:A:LYS:HB2	7	0.16
(1,962)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	4	0.16
(1,962)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	9	0.16
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	8	0.16
(1,956)	1:97:A:ARG:HG2	1:97:A:ARG:HA	8	0.16
(1,956)	1:97:A:ARG:HG3	1:97:A:ARG:HA	8	0.16
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	7	0.16
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	7	0.16
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	7	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	2	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	2	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	4	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	4	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	6	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	6	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	7	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	7	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	10	0.16
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	10	0.16
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	8	0.16
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	8	0.16
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	8	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	5	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	5	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	5	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	9	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	9	0.16
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	9	0.16
(1,817)	1:82:A:GLU:HA	1:85:A:ILE:HG12	1	0.16
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD11	6	0.16
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD12	6	0.16
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD13	6	0.16
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD21	6	0.16
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD22	6	0.16
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD23	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	2	0.16
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	2	0.16
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	2	0.16
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	4	0.16
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	4	0.16
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	4	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG21	4	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG22	4	0.16
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG23	4	0.16
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	2	0.16
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	2	0.16
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	3	0.16
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	10	0.16
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	10	0.16
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	10	0.16
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	6	0.16
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	6	0.16
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	6	0.16
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	1	0.16
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	2	0.16
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	8	0.16
(1,207)	1:25:A:LEU:HG	1:89:A:VAL:HG11	9	0.16
(1,207)	1:25:A:LEU:HG	1:89:A:VAL:HG12	9	0.16
(1,207)	1:25:A:LEU:HG	1:89:A:VAL:HG13	9	0.16
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	6	0.16
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	6	0.16
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	6	0.16
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	5	0.16
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	5	0.16
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	5	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	5	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	5	0.16
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	5	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	5	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	5	0.16
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	5	0.16
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD21	9	0.16
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD22	9	0.16
(1,97)	1:12:A:LYS:HG2	1:35:A:LEU:HD23	9	0.16
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD21	9	0.16
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD22	9	0.16
(1,97)	1:12:A:LYS:HG3	1:35:A:LEU:HD23	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	4	0.16
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	8	0.16
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	7	0.16
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	8	0.16
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	10	0.16
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	3	0.16
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	3	0.16
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	6	0.16
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	6	0.16
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	7	0.16
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	7	0.16
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	6	0.15
(2,29)	1:31:A:ALA:O	1:35:A:LEU:H	4	0.15
(2,20)	1:14:A:VAL:O	1:18:A:PHE:N	10	0.15
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	3	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	6	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	6	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	6	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	10	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	10	0.15
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	10	0.15
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	1	0.15
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	2	0.15
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	7	0.15
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	2	0.15
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	10	0.15
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	10	0.15
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	10	0.15
(1,3074)	1:115:A:THR:HA	1:116:A:LEU:H	10	0.15
(1,3064)	1:114:A:ARG:H	1:115:A:THR:HA	1	0.15
(1,3064)	1:114:A:ARG:H	1:115:A:THR:HA	6	0.15
(1,3046)	1:112:A:GLN:HA	1:113:A:GLY:H	6	0.15
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	7	0.15
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	8	0.15
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	1	0.15
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	8	0.15
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	4	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	1	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	1	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	1	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	10	0.15
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	10	0.15
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	1	0.15
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	3	0.15
(1,2804)	1:101:A:THR:HA	1:103:A:LEU:H	6	0.15
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	5	0.15
(1,2765)	1:98:A:LYS:HG3	1:98:A:LYS:H	4	0.15
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	10	0.15
(1,2749)	1:97:A:ARG:HG2	1:97:A:ARG:HE	3	0.15
(1,2749)	1:97:A:ARG:HG2	1:97:A:ARG:HE	8	0.15
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	10	0.15
(1,2738)	1:96:A:LYS:HG3	1:97:A:ARG:H	10	0.15
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	9	0.15
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	5	0.15
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	6	0.15
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	7	0.15
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	9	0.15
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	10	0.15
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	4	0.15
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	9	0.15
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	7	0.15
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	3	0.15
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	6	0.15
(1,2580)	1:89:A:VAL:H	1:90:A:THR:HB	5	0.15
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	2	0.15
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	10	0.15
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	4	0.15
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	4	0.15
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	5	0.15
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	7	0.15
(1,2424)	1:82:A:GLU:HG2	1:83:A:SER:H	9	0.15
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	2	0.15
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	6	0.15
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	8	0.15
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	9	0.15
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	1	0.15
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	10	0.15
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	6	0.15
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	8	0.15
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	9	0.15
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	1	0.15
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	7	0.15
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	4	0.15
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	7	0.15
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	9	0.15
(1,2163)	1:68:A:LEU:HG	1:68:A:LEU:H	9	0.15
(1,2087)	1:57:A:LEU:HA	1:58:A:VAL:H	7	0.15
(1,2084)	1:57:A:LEU:HG	1:57:A:LEU:H	7	0.15
(1,2052)	1:53:A:LEU:HG	1:54:A:ALA:H	9	0.15
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	2	0.15
(1,2018)	1:51:A:ASN:HD22	1:52:A:LEU:HD11	5	0.15
(1,2018)	1:51:A:ASN:HD22	1:52:A:LEU:HD12	5	0.15
(1,2018)	1:51:A:ASN:HD22	1:52:A:LEU:HD13	5	0.15
(1,2005)	1:51:A:ASN:HB2	1:51:A:ASN:H	9	0.15
(1,1964)	1:47:A:LEU:H	1:50:A:THR:H	3	0.15
(1,1870)	1:43:A:LEU:HB3	1:44:A:VAL:H	5	0.15
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	6	0.15
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	7	0.15
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	7	0.15
(1,1745)	1:36:A:GLN:HB2	1:36:A:GLN:HE21	10	0.15
(1,1745)	1:36:A:GLN:HB3	1:36:A:GLN:HE21	10	0.15
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	5	0.15
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	7	0.15
(1,1635)	1:31:A:ALA:H	1:32:A:ILE:HG12	6	0.15
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	6	0.15
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	10	0.15
(1,1611)	1:30:A:MET:HG2	1:30:A:MET:H	2	0.15
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	7	0.15
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	10	0.15
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	8	0.15
(1,1514)	1:25:A:LEU:HB3	1:27:A:TRP:H	4	0.15
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	3	0.15
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	10	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	5	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	5	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	5	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG21	9	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG22	9	0.15
(1,1486)	1:23:A:GLN:HE22	1:85:A:ILE:HG23	9	0.15
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	4	0.15
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	4	0.15
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	4	0.15
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	7	0.15
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	4	0.15
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	5	0.15
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	6	0.15
(1,1310)	1:13:A:GLU:HG3	1:16:A:ASP:H	8	0.15
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	3	0.15
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	3	0.15
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	3	0.15
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	4	0.15
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	4	0.15
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	4	0.15
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	5	0.15
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	5	0.15
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	5	0.15
(1,1216)	1:9:A:ARG:H	1:11:A:VAL:H	6	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	4	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	4	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	5	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	5	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	9	0.15
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	9	0.15
(1,1152)	1:117:A:TYR:HB2	1:119:A:PHE:HB3	6	0.15
(1,1133)	1:116:A:LEU:HA	1:116:A:LEU:HG	1	0.15
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	6	0.15
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	6	0.15
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	6	0.15
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	6	0.15
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	6	0.15
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	6	0.15
(1,991)	1:103:A:LEU:HD11	1:103:A:LEU:HA	5	0.15
(1,991)	1:103:A:LEU:HD12	1:103:A:LEU:HA	5	0.15
(1,991)	1:103:A:LEU:HD13	1:103:A:LEU:HA	5	0.15
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	3	0.15
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	3	0.15
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	3	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	3	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	3	0.15
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	3	0.15
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	3	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	1	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	1	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	3	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	5	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	5	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	8	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	8	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD1	9	0.15
(1,900)	1:91:A:TYR:HB2	1:91:A:TYR:HD2	9	0.15
(1,868)	1:87:A:ASP:HB3	1:104:A:ASP:HB3	4	0.15
(1,868)	1:87:A:ASP:HB3	1:104:A:ASP:HB3	5	0.15
(1,862)	1:86:A:ARG:HD3	1:86:A:ARG:HB3	8	0.15
(1,860)	1:85:A:ILE:HG12	1:100:A:VAL:HG11	1	0.15
(1,860)	1:85:A:ILE:HG12	1:100:A:VAL:HG12	1	0.15
(1,860)	1:85:A:ILE:HG12	1:100:A:VAL:HG13	1	0.15
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	1	0.15
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	1	0.15
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	1	0.15
(1,806)	1:81:A:LEU:HA	1:84:A:VAL:HB	1	0.15
(1,803)	1:81:A:LEU:HA	1:84:A:VAL:HB	1	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	2	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	2	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	2	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	2	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	2	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	2	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	4	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	4	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	4	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	4	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	4	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	4	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	6	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	6	0.15
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	6	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	6	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	6	0.15
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	6	0.15
(1,652)	1:69:A:ILE:HG21	1:73:A:VAL:HG11	5	0.15
(1,652)	1:69:A:ILE:HG21	1:73:A:VAL:HG12	5	0.15
(1,652)	1:69:A:ILE:HG21	1:73:A:VAL:HG13	5	0.15
(1,652)	1:69:A:ILE:HG22	1:73:A:VAL:HG11	5	0.15
(1,652)	1:69:A:ILE:HG22	1:73:A:VAL:HG12	5	0.15
(1,652)	1:69:A:ILE:HG22	1:73:A:VAL:HG13	5	0.15
(1,652)	1:69:A:ILE:HG23	1:73:A:VAL:HG11	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:69:A:ILE:HG23	1:73:A:VAL:HG12	5	0.15
(1,652)	1:69:A:ILE:HG23	1:73:A:VAL:HG13	5	0.15
(1,637)	1:68:A:LEU:HG	1:68:A:LEU:HA	9	0.15
(1,607)	1:60:A:ARG:HA	1:62:A:SER:HB2	2	0.15
(1,575)	1:58:A:VAL:HA	1:59:A:PRO:HB2	8	0.15
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB1	3	0.15
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB2	3	0.15
(1,535)	1:52:A:LEU:HD21	1:54:A:ALA:HB3	3	0.15
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB1	3	0.15
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB2	3	0.15
(1,535)	1:52:A:LEU:HD22	1:54:A:ALA:HB3	3	0.15
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB1	3	0.15
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB2	3	0.15
(1,535)	1:52:A:LEU:HD23	1:54:A:ALA:HB3	3	0.15
(1,513)	1:47:A:LEU:HD21	1:50:A:THR:HG21	6	0.15
(1,513)	1:47:A:LEU:HD21	1:50:A:THR:HG22	6	0.15
(1,513)	1:47:A:LEU:HD21	1:50:A:THR:HG23	6	0.15
(1,513)	1:47:A:LEU:HD22	1:50:A:THR:HG21	6	0.15
(1,513)	1:47:A:LEU:HD22	1:50:A:THR:HG22	6	0.15
(1,513)	1:47:A:LEU:HD22	1:50:A:THR:HG23	6	0.15
(1,513)	1:47:A:LEU:HD23	1:50:A:THR:HG21	6	0.15
(1,513)	1:47:A:LEU:HD23	1:50:A:THR:HG22	6	0.15
(1,513)	1:47:A:LEU:HD23	1:50:A:THR:HG23	6	0.15
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	5	0.15
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	8	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	1	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	1	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	1	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	5	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	5	0.15
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	5	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	6	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	6	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	6	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	7	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	7	0.15
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	7	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD11	3	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD12	3	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD13	3	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD11	5	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD12	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD13	5	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD11	10	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD12	10	0.15
(1,361)	1:35:A:LEU:HB3	1:35:A:LEU:HD13	10	0.15
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	4	0.15
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	3	0.15
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	7	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	5	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	5	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	5	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	8	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	8	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	8	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	10	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	10	0.15
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	10	0.15
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	9	0.15
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	6	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	1	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	1	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	2	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	2	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	3	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	3	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	6	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	6	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	7	0.15
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	7	0.15
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	7	0.15
(1,213)	1:25:A:LEU:HB2	1:98:A:LYS:HB3	9	0.15
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	8	0.15
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	8	0.15
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	8	0.15
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	8	0.15
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	8	0.15
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	8	0.15
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	8	0.15
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	8	0.15
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	8	0.15
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	7	0.15
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	7	0.15
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	8	0.15
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	8	0.15
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	8	0.15
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	2	0.15
(1,172)	1:21:A:LYS:HD2	1:85:A:ILE:HG12	8	0.15
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	5	0.15
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	6	0.15
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	6	0.15
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	8	0.15
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	8	0.15
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	8	0.15
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	4	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	1	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	1	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	4	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	4	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	9	0.15
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	9	0.15
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	4	0.15
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	4	0.15
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	4	0.15
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD11	5	0.15
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD12	5	0.15
(1,4)	1:2:A:ILE:HA	1:2:A:ILE:HD13	5	0.15
(2,50)	1:41:A:ALA:O	1:45:A:GLY:N	8	0.14
(2,32)	1:32:A:ILE:O	1:36:A:GLN:N	4	0.14
(2,26)	1:29:A:SER:O	1:33:A:MET:N	4	0.14
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	1	0.14
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	4	0.14
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	6	0.14
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	8	0.14
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	6	0.14
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	4	0.14
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	4	0.14
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	4	0.14
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	9	0.14
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	10	0.14
(1,3169)	1:41:A:ALA:HB1	1:80:A:PHE:HZ	6	0.14
(1,3169)	1:41:A:ALA:HB2	1:80:A:PHE:HZ	6	0.14
(1,3169)	1:41:A:ALA:HB3	1:80:A:PHE:HZ	6	0.14
(1,3165)	1:34:A:ALA:HA	1:80:A:PHE:HZ	4	0.14
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	3	0.14
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	5	0.14
(1,3158)	1:27:A:TRP:HE3	1:31:A:ALA:HA	10	0.14
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	7	0.14
(1,3130)	1:15:A:THR:HA	1:18:A:PHE:HZ	4	0.14
(1,3124)	1:120:A:GLY:HA3	1:121:A:GLY:H	4	0.14
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	4	0.14
(1,3084)	1:116:A:LEU:HD21	1:116:A:LEU:H	10	0.14
(1,3084)	1:116:A:LEU:HD22	1:116:A:LEU:H	10	0.14
(1,3084)	1:116:A:LEU:HD23	1:116:A:LEU:H	10	0.14
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	1	0.14
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	5	0.14
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	8	0.14
(1,3017)	1:111:A:ARG:H	1:112:A:GLN:HB3	2	0.14
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	2	0.14
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	4	0.14
(1,2950)	1:107:A:TYR:H	1:110:A:LYS:HB2	10	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	2	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	2	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	2	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	3	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	3	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	3	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	6	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	6	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	6	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	7	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	7	0.14
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	7	0.14
(1,2862)	1:103:A:LEU:HB3	1:107:A:TYR:H	8	0.14
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	8	0.14
(1,2813)	1:101:A:THR:H	1:104:A:ASP:HB3	9	0.14
(1,2752)	1:97:A:ARG:H	1:98:A:LYS:HA	2	0.14
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	8	0.14
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	5	0.14
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	6	0.14
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	7	0.14
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	10	0.14
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	4	0.14
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	7	0.14
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	8	0.14
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	5	0.14
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	1	0.14
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	5	0.14
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	10	0.14
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	6	0.14
(1,2542)	1:87:A:ASP:HB3	1:88:A:SER:H	5	0.14
(1,2509)	1:85:A:ILE:HB	1:88:A:SER:H	8	0.14
(1,2489)	1:85:A:ILE:HD11	1:85:A:ILE:H	8	0.14
(1,2489)	1:85:A:ILE:HD12	1:85:A:ILE:H	8	0.14
(1,2489)	1:85:A:ILE:HD13	1:85:A:ILE:H	8	0.14
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	1	0.14
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	1	0.14
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	1	0.14
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	8	0.14
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	8	0.14
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	8	0.14
(1,2386)	1:80:A:PHE:HD1	1:112:A:GLN:HE22	3	0.14
(1,2386)	1:80:A:PHE:HD2	1:112:A:GLN:HE22	3	0.14
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	1	0.14
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	3	0.14
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	4	0.14
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	7	0.14
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	10	0.14
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	2	0.14
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	6	0.14
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	7	0.14
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	6	0.14
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	2	0.14
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	3	0.14
(1,2163)	1:68:A:LEU:HG	1:68:A:LEU:H	7	0.14
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	8	0.14
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	9	0.14
(1,2090)	1:57:A:LEU:HG	1:58:A:VAL:H	1	0.14
(1,2075)	1:56:A:HIS:H	1:57:A:LEU:H	5	0.14
(1,2071)	1:55:A:LEU:H	1:57:A:LEU:H	4	0.14
(1,2071)	1:55:A:LEU:H	1:57:A:LEU:H	7	0.14
(1,2047)	1:53:A:LEU:HG	1:53:A:LEU:H	9	0.14
(1,2038)	1:52:A:LEU:HG	1:52:A:LEU:H	9	0.14
(1,2026)	1:51:A:ASN:HB3	1:53:A:LEU:H	8	0.14
(1,2013)	1:51:A:ASN:HB2	1:52:A:LEU:H	4	0.14
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	4	0.14
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	5	0.14
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	10	0.14
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	3	0.14
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	3	0.14
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	9	0.14
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	1	0.14
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	3	0.14
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	4	0.14
(1,1581)	1:28:A:GLN:HG2	1:28:A:GLN:HE21	5	0.14
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	2	0.14
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	9	0.14
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	1	0.14
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	1	0.14
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	3	0.14
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	3	0.14
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	10	0.14
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	10	0.14
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	3	0.14
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	8	0.14
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	7	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	3	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	3	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	3	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	6	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	6	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	6	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	9	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	9	0.14
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	9	0.14
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	3	0.14
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	2	0.14
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	2	0.14
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	2	0.14
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	10	0.14
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	10	0.14
(1,1441)	1:21:A:LYS:HB2	1:24:A:ASP:H	10	0.14
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	3	0.14
(1,1245)	1:11:A:VAL:HG11	1:11:A:VAL:H	10	0.14
(1,1245)	1:11:A:VAL:HG12	1:11:A:VAL:H	10	0.14
(1,1245)	1:11:A:VAL:HG13	1:11:A:VAL:H	10	0.14
(1,1219)	1:9:A:ARG:H	1:12:A:LYS:H	9	0.14
(1,1218)	1:9:A:ARG:HB2	1:11:A:VAL:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:9:A:ARG:H	1:11:A:VAL:H	8	0.14
(1,1216)	1:9:A:ARG:H	1:11:A:VAL:H	9	0.14
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	5	0.14
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	7	0.14
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	9	0.14
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	3	0.14
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	3	0.14
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD1	7	0.14
(1,1155)	1:119:A:PHE:HB2	1:119:A:PHE:HD2	7	0.14
(1,1037)	1:106:A:VAL:HG21	1:109:A:LEU:HB3	10	0.14
(1,1037)	1:106:A:VAL:HG22	1:109:A:LEU:HB3	10	0.14
(1,1037)	1:106:A:VAL:HG23	1:109:A:LEU:HB3	10	0.14
(1,1024)	1:105:A:VAL:HG11	1:109:A:LEU:HB3	9	0.14
(1,1024)	1:105:A:VAL:HG12	1:109:A:LEU:HB3	9	0.14
(1,1024)	1:105:A:VAL:HG13	1:109:A:LEU:HB3	9	0.14
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	7	0.14
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	7	0.14
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	7	0.14
(1,991)	1:103:A:LEU:HD11	1:103:A:LEU:HA	10	0.14
(1,991)	1:103:A:LEU:HD12	1:103:A:LEU:HA	10	0.14
(1,991)	1:103:A:LEU:HD13	1:103:A:LEU:HA	10	0.14
(1,968)	1:98:A:LYS:HA	1:98:A:LYS:HG2	4	0.14
(1,968)	1:98:A:LYS:HA	1:98:A:LYS:HG2	5	0.14
(1,968)	1:98:A:LYS:HA	1:98:A:LYS:HG2	9	0.14
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	6	0.14
(1,950)	1:96:A:LYS:HD3	1:96:A:LYS:HB2	1	0.14
(1,868)	1:87:A:ASP:HB3	1:104:A:ASP:HB3	9	0.14
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	2	0.14
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	2	0.14
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	2	0.14
(1,816)	1:82:A:GLU:HA	1:85:A:ILE:HG13	8	0.14
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	3	0.14
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	3	0.14
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	3	0.14
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	3	0.14
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	3	0.14
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	3	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG2	2	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG3	2	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG2	2	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG3	2	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG3	2	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG2	4	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG3	4	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG2	4	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG3	4	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG2	4	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG3	4	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG2	10	0.14
(1,683)	1:73:A:VAL:HG11	1:74:A:ARG:HG3	10	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG2	10	0.14
(1,683)	1:73:A:VAL:HG12	1:74:A:ARG:HG3	10	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG2	10	0.14
(1,683)	1:73:A:VAL:HG13	1:74:A:ARG:HG3	10	0.14
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	1	0.14
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	1	0.14
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	8	0.14
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	8	0.14
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	9	0.14
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	9	0.14
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	9	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	4	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	4	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	4	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	9	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	9	0.14
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	9	0.14
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	1	0.14
(1,455)	1:43:A:LEU:HB3	1:47:A:LEU:HB3	9	0.14
(1,454)	1:43:A:LEU:HA	1:47:A:LEU:HB3	6	0.14
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	8	0.14
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	8	0.14
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	8	0.14
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	2	0.14
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	2	0.14
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	2	0.14
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	4	0.14
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	4	0.14
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	4	0.14
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	8	0.14
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	8	0.14
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	8	0.14
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	8	0.14
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	8	0.14
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	8	0.14
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	8	0.14
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	8	0.14
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	3	0.14
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	6	0.14
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	2	0.14
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	8	0.14
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	9	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	3	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	3	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	3	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	9	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	9	0.14
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	9	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	3	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	3	0.14
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	3	0.14
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	1	0.14
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	1	0.14
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	3	0.14
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	7	0.14
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	3	0.14
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	3	0.14
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	3	0.14
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	3	0.14
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	3	0.14
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	3	0.14
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	3	0.14
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	3	0.14
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	3	0.14
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	1	0.14
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	3	0.14
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	6	0.14
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	10	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	3	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	3	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	3	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	3	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	3	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	3	0.14
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	3	0.14
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	3	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	10	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	10	0.14
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	10	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	10	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	10	0.14
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	10	0.14
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	10	0.14
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	10	0.14
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	10	0.14
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	2	0.14
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	3	0.14
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	1	0.14
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	1	0.14
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	2	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	6	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	6	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	6	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	9	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	9	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	9	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	10	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	10	0.14
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	10	0.14
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	8	0.14
(1,51)	1:9:A:ARG:HB2	1:13:A:GLU:HB2	9	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	7	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	7	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	8	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	8	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG2	10	0.14
(1,36)	1:9:A:ARG:HA	1:9:A:ARG:HG3	10	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	1	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	1	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	1	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	9	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	9	0.14
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	9	0.14
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	10	0.13
(2,48)	1:40:A:GLU:O	1:44:A:VAL:N	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	5	0.13
(2,2)	1:5:A:ILE:O	1:9:A:ARG:N	9	0.13
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	2	0.13
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	2	0.13
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	2	0.13
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	5	0.13
(1,3189)	1:80:A:PHE:HZ	1:81:A:LEU:HA	8	0.13
(1,3166)	1:38:A:ALA:HA	1:80:A:PHE:HZ	8	0.13
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	5	0.13
(1,3162)	1:27:A:TRP:HD1	1:100:A:VAL:HB	6	0.13
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	8	0.13
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	1	0.13
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	7	0.13
(1,3099)	1:117:A:TYR:HB3	1:118:A:GLY:H	5	0.13
(1,3091)	1:116:A:LEU:HB3	1:117:A:TYR:H	10	0.13
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	5	0.13
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	5	0.13
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	5	0.13
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	9	0.13
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	9	0.13
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	9	0.13
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	9	0.13
(1,3036)	1:112:A:GLN:HB2	1:112:A:GLN:HE21	1	0.13
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	1	0.13
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	4	0.13
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	10	0.13
(1,2980)	1:109:A:LEU:HA	1:112:A:GLN:H	4	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	4	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	4	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	4	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG11	9	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG12	9	0.13
(1,2892)	1:105:A:VAL:H	1:106:A:VAL:HG13	9	0.13
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	4	0.13
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	4	0.13
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	8	0.13
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	3	0.13
(1,2711)	1:94:A:HIS:HB2	1:95:A:ALA:H	8	0.13
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	2	0.13
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	5	0.13
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	1	0.13
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	3	0.13
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	6	0.13
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	3	0.13
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	6	0.13
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	7	0.13
(1,2584)	1:89:A:VAL:HB	1:90:A:THR:H	8	0.13
(1,2466)	1:84:A:VAL:H	1:86:A:ARG:HB3	8	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	2	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	2	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	2	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	4	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	4	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	4	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	5	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	5	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	5	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	6	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	6	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	6	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	7	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	7	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	7	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	9	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	9	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	9	0.13
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	10	0.13
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	10	0.13
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	10	0.13
(1,2386)	1:80:A:PHE:HD1	1:112:A:GLN:HE22	4	0.13
(1,2386)	1:80:A:PHE:HD2	1:112:A:GLN:HE22	4	0.13
(1,2312)	1:78:A:LYS:HG2	1:78:A:LYS:H	5	0.13
(1,2305)	1:77:A:LEU:HB2	1:81:A:LEU:H	3	0.13
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	4	0.13
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	4	0.13
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	4	0.13
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	4	0.13
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	9	0.13
(1,2219)	1:73:A:VAL:HB	1:74:A:ARG:H	9	0.13
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	1	0.13
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	1	0.13
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	1	0.13
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	8	0.13
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	8	0.13
(1,2167)	1:68:A:LEU:HB2	1:69:A:ILE:H	5	0.13
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	8	0.13
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	10	0.13
(1,2156)	1:66:A:SER:HB2	1:68:A:LEU:H	3	0.13
(1,2156)	1:66:A:SER:HB2	1:68:A:LEU:H	7	0.13
(1,2152)	1:65:A:ILE:H	1:66:A:SER:HA	1	0.13
(1,2143)	1:65:A:ILE:HB	1:65:A:ILE:H	3	0.13
(1,2136)	1:64:A:ARG:HA	1:65:A:ILE:H	2	0.13
(1,2136)	1:64:A:ARG:HA	1:65:A:ILE:H	6	0.13
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	1	0.13
(1,2090)	1:57:A:LEU:HG	1:58:A:VAL:H	2	0.13
(1,2083)	1:57:A:LEU:HD11	1:57:A:LEU:H	7	0.13
(1,2083)	1:57:A:LEU:HD12	1:57:A:LEU:H	7	0.13
(1,2083)	1:57:A:LEU:HD13	1:57:A:LEU:H	7	0.13
(1,2068)	1:55:A:LEU:H	1:56:A:HIS:HB2	5	0.13
(1,2038)	1:52:A:LEU:HG	1:52:A:LEU:H	8	0.13
(1,1997)	1:50:A:THR:HA	1:51:A:ASN:H	3	0.13
(1,1987)	1:49:A:HIS:HB3	1:49:A:HIS:H	5	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	1	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	1	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	1	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	2	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	2	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	2	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	3	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	3	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	3	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	5	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	5	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	5	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	6	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	6	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	6	0.13
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	7	0.13
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	7	0.13
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	7	0.13
(1,1803)	1:39:A:SER:HA	1:42:A:TYR:H	6	0.13
(1,1788)	1:38:A:ALA:HA	1:41:A:ALA:H	5	0.13
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	8	0.13
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:34:A:ALA:HA	1:37:A:GLU:H	2	0.13
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	8	0.13
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	9	0.13
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	4	0.13
(1,1612)	1:30:A:MET:HG3	1:30:A:MET:H	8	0.13
(1,1600)	1:28:A:GLN:H	1:100:A:VAL:HB	5	0.13
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	6	0.13
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	3	0.13
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	7	0.13
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	7	0.13
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	7	0.13
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	9	0.13
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	9	0.13
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	1	0.13
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	1	0.13
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	5	0.13
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	6	0.13
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	1	0.13
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	4	0.13
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	4	0.13
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	2	0.13
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	2	0.13
(1,1372)	1:17:A:GLU:HG2	1:17:A:GLU:H	4	0.13
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	3	0.13
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	3	0.13
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	3	0.13
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	5	0.13
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	5	0.13
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	5	0.13
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	7	0.13
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	7	0.13
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	7	0.13
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	10	0.13
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	10	0.13
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	10	0.13
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	1	0.13
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	1	0.13
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	8	0.13
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	8	0.13
(1,1219)	1:9:A:ARG:H	1:12:A:LYS:H	8	0.13
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	3	0.13
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:120:A:GLY:HA2	1:121:A:GLY:HA2	8	0.13
(1,1133)	1:116:A:LEU:HA	1:116:A:LEU:HG	3	0.13
(1,1128)	1:115:A:THR:HA	1:117:A:TYR:HA	3	0.13
(1,1114)	1:114:A:ARG:HD2	1:114:A:ARG:HA	9	0.13
(1,1110)	1:113:A:GLY:HA2	1:114:A:ARG:HG3	10	0.13
(1,1081)	1:110:A:LYS:HA	1:110:A:LYS:HG3	7	0.13
(1,1033)	1:106:A:VAL:HA	1:109:A:LEU:HB2	4	0.13
(1,1010)	1:104:A:ASP:HA	1:107:A:TYR:HD2	4	0.13
(1,1005)	1:103:A:LEU:HD11	1:107:A:TYR:HE2	1	0.13
(1,1005)	1:103:A:LEU:HD12	1:107:A:TYR:HE2	1	0.13
(1,1005)	1:103:A:LEU:HD13	1:107:A:TYR:HE2	1	0.13
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	1	0.13
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	1	0.13
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	1	0.13
(1,964)	1:98:A:LYS:HD2	1:98:A:LYS:HB2	2	0.13
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	7	0.13
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD11	4	0.13
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD12	4	0.13
(1,849)	1:85:A:ILE:HB	1:85:A:ILE:HD13	4	0.13
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB1	7	0.13
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB2	7	0.13
(1,823)	1:83:A:SER:HB2	1:108:A:ALA:HB3	7	0.13
(1,806)	1:81:A:LEU:HA	1:84:A:VAL:HB	8	0.13
(1,803)	1:81:A:LEU:HA	1:84:A:VAL:HB	8	0.13
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG21	9	0.13
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG22	9	0.13
(1,792)	1:80:A:PHE:HE1	1:84:A:VAL:HG23	9	0.13
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG21	9	0.13
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG22	9	0.13
(1,792)	1:80:A:PHE:HE2	1:84:A:VAL:HG23	9	0.13
(1,719)	1:75:A:ALA:HA	1:77:A:LEU:HB2	2	0.13
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD2	8	0.13
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD3	8	0.13
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD11	6	0.13
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD12	6	0.13
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD13	6	0.13
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD11	6	0.13
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD12	6	0.13
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD13	6	0.13
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD11	6	0.13
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD12	6	0.13
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:68:A:LEU:HB3	1:71:A:GLU:HA	1	0.13
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG21	2	0.13
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG22	2	0.13
(1,644)	1:68:A:LEU:HB3	1:69:A:ILE:HG23	2	0.13
(1,637)	1:68:A:LEU:HG	1:68:A:LEU:HA	3	0.13
(1,637)	1:68:A:LEU:HG	1:68:A:LEU:HA	7	0.13
(1,631)	1:65:A:ILE:HG21	1:68:A:LEU:HA	6	0.13
(1,631)	1:65:A:ILE:HG22	1:68:A:LEU:HA	6	0.13
(1,631)	1:65:A:ILE:HG23	1:68:A:LEU:HA	6	0.13
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	6	0.13
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	6	0.13
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	6	0.13
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD11	1	0.13
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD12	1	0.13
(1,554)	1:54:A:ALA:HA	1:57:A:LEU:HD13	1	0.13
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD21	9	0.13
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD22	9	0.13
(1,540)	1:53:A:LEU:HA	1:53:A:LEU:HD23	9	0.13
(1,532)	1:52:A:LEU:HD21	1:52:A:LEU:HB3	5	0.13
(1,532)	1:52:A:LEU:HD22	1:52:A:LEU:HB3	5	0.13
(1,532)	1:52:A:LEU:HD23	1:52:A:LEU:HB3	5	0.13
(1,521)	1:50:A:THR:HA	1:53:A:LEU:HD11	1	0.13
(1,521)	1:50:A:THR:HA	1:53:A:LEU:HD12	1	0.13
(1,521)	1:50:A:THR:HA	1:53:A:LEU:HD13	1	0.13
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD11	10	0.13
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD12	10	0.13
(1,460)	1:44:A:VAL:HA	1:47:A:LEU:HD13	10	0.13
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	9	0.13
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	4	0.13
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	4	0.13
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	4	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	1	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	1	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	1	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	3	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	3	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	3	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD11	4	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD12	4	0.13
(1,433)	1:43:A:LEU:HB2	1:43:A:LEU:HD13	4	0.13
(1,338)	1:32:A:ILE:HA	1:35:A:LEU:HD21	9	0.13
(1,338)	1:32:A:ILE:HA	1:35:A:LEU:HD22	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:32:A:ILE:HA	1:35:A:LEU:HD23	9	0.13
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	3	0.13
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	3	0.13
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	3	0.13
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	5	0.13
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	5	0.13
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	5	0.13
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	6	0.13
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	6	0.13
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	6	0.13
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	9	0.13
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	9	0.13
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	9	0.13
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	3	0.13
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	3	0.13
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	3	0.13
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	3	0.13
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	3	0.13
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	3	0.13
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	3	0.13
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	3	0.13
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	3	0.13
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	10	0.13
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	5	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	1	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	1	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	1	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	6	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	6	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	6	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	7	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	7	0.13
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	7	0.13
(1,282)	1:28:A:GLN:HG3	1:99:A:THR:HA	2	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	4	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	4	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	4	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	6	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	6	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	6	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	7	0.13
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	7	0.13
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	3	0.13
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	6	0.13
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	5	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	5	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	5	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	8	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	8	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	9	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	9	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	10	0.13
(1,233)	1:26:A:ARG:HD2	1:26:A:ARG:HB3	10	0.13
(1,230)	1:26:A:ARG:HB2	1:26:A:ARG:HD3	10	0.13
(1,230)	1:26:A:ARG:HB3	1:26:A:ARG:HD3	10	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	5	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	5	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	5	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	5	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	5	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	5	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	5	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	5	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	5	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	6	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	6	0.13
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	6	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	6	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	6	0.13
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	6	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	6	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	6	0.13
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	6	0.13
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	2	0.13
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	2	0.13
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	2	0.13
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	7	0.13
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	8	0.13
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	3	0.13
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD11	9	0.13
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD12	9	0.13
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD13	9	0.13
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG11	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG12	6	0.13
(1,153)	1:19:A:THR:HG21	1:89:A:VAL:HG13	6	0.13
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG11	6	0.13
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG12	6	0.13
(1,153)	1:19:A:THR:HG22	1:89:A:VAL:HG13	6	0.13
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG11	6	0.13
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG12	6	0.13
(1,153)	1:19:A:THR:HG23	1:89:A:VAL:HG13	6	0.13
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG21	8	0.13
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG22	8	0.13
(1,130)	1:15:A:THR:HA	1:15:A:THR:HG23	8	0.13
(1,112)	1:14:A:VAL:HG21	1:17:A:GLU:HB2	4	0.13
(1,112)	1:14:A:VAL:HG22	1:17:A:GLU:HB2	4	0.13
(1,112)	1:14:A:VAL:HG23	1:17:A:GLU:HB2	4	0.13
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	3	0.13
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	3	0.13
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	3	0.13
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	5	0.13
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	5	0.13
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	5	0.13
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	6	0.13
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	6	0.13
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	6	0.13
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	8	0.13
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	8	0.13
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	8	0.13
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	9	0.13
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	9	0.13
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	9	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	1	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	1	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	1	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	2	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	2	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	2	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	4	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	4	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	4	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	5	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	5	0.13
(1,55)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	5	0.13
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	2	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	2	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	2	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	3	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	3	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	3	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	4	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	4	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	4	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	5	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	5	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	5	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	8	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	8	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	8	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	10	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	10	0.13
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	10	0.13
(1,1)	1:2:A:ILE:HG13	1:2:A:ILE:HA	2	0.13
(1,1)	1:2:A:ILE:HG13	1:2:A:ILE:HA	6	0.13
(2,95)	1:86:A:ARG:O	1:90:A:THR:H	9	0.12
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	3	0.12
(1,3212)	1:118:A:GLY:HA2	1:119:A:PHE:HD1	4	0.12
(1,3212)	1:118:A:GLY:HA2	1:119:A:PHE:HD2	4	0.12
(1,3203)	1:80:A:PHE:HE1	1:112:A:GLN:HB2	9	0.12
(1,3203)	1:80:A:PHE:HE1	1:112:A:GLN:HB3	9	0.12
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	5	0.12
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	5	0.12
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	5	0.12
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	6	0.12
(1,3130)	1:15:A:THR:HA	1:18:A:PHE:HZ	2	0.12
(1,3106)	1:118:A:GLY:HA3	1:119:A:PHE:H	2	0.12
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	4	0.12
(1,3099)	1:117:A:TYR:HB3	1:118:A:GLY:H	9	0.12
(1,3095)	1:117:A:TYR:HB3	1:117:A:TYR:H	8	0.12
(1,3095)	1:117:A:TYR:HB3	1:117:A:TYR:H	10	0.12
(1,3092)	1:116:A:LEU:HB3	1:118:A:GLY:H	2	0.12
(1,3036)	1:112:A:GLN:HB2	1:112:A:GLN:HE21	5	0.12
(1,3036)	1:112:A:GLN:HB2	1:112:A:GLN:HE21	6	0.12
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	3	0.12
(1,3008)	1:110:A:LYS:HE2	1:116:A:LEU:H	7	0.12
(1,3008)	1:110:A:LYS:HE3	1:116:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3005)	1:110:A:LYS:HB3	1:113:A:GLY:H	5	0.12
(1,2939)	1:107:A:TYR:HB3	1:108:A:ALA:H	4	0.12
(1,2939)	1:107:A:TYR:HB3	1:108:A:ALA:H	9	0.12
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	6	0.12
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	9	0.12
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	10	0.12
(1,2804)	1:101:A:THR:HA	1:103:A:LEU:H	1	0.12
(1,2804)	1:101:A:THR:HA	1:103:A:LEU:H	7	0.12
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	6	0.12
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	1	0.12
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	10	0.12
(1,2765)	1:98:A:LYS:HG3	1:98:A:LYS:H	5	0.12
(1,2761)	1:97:A:ARG:HB3	1:99:A:THR:H	2	0.12
(1,2747)	1:97:A:ARG:HB2	1:97:A:ARG:HE	2	0.12
(1,2747)	1:97:A:ARG:HB3	1:97:A:ARG:HE	2	0.12
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	8	0.12
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	9	0.12
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	2	0.12
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	4	0.12
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	3	0.12
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	4	0.12
(1,2659)	1:92:A:THR:HA	1:95:A:ALA:H	9	0.12
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	2	0.12
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	8	0.12
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	9	0.12
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	5	0.12
(1,2620)	1:91:A:TYR:H	1:92:A:THR:HA	7	0.12
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	2	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	1	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	1	0.12
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	1	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	2	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	2	0.12
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	2	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	3	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	3	0.12
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	3	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	8	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	8	0.12
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	8	0.12
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	10	0.12
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	10	0.12
(1,2576)	1:89:A:VAL:HG21	1:89:A:VAL:H	9	0.12
(1,2576)	1:89:A:VAL:HG22	1:89:A:VAL:H	9	0.12
(1,2576)	1:89:A:VAL:HG23	1:89:A:VAL:H	9	0.12
(1,2484)	1:84:A:VAL:HA	1:112:A:GLN:HE21	1	0.12
(1,2484)	1:84:A:VAL:HA	1:112:A:GLN:HE21	10	0.12
(1,2460)	1:84:A:VAL:HG11	1:84:A:VAL:H	3	0.12
(1,2460)	1:84:A:VAL:HG12	1:84:A:VAL:H	3	0.12
(1,2460)	1:84:A:VAL:HG13	1:84:A:VAL:H	3	0.12
(1,2445)	1:83:A:SER:HB2	1:84:A:VAL:H	5	0.12
(1,2445)	1:83:A:SER:HB2	1:84:A:VAL:H	9	0.12
(1,2383)	1:80:A:PHE:HD1	1:112:A:GLN:HE21	7	0.12
(1,2383)	1:80:A:PHE:HD2	1:112:A:GLN:HE21	7	0.12
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	2	0.12
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	2	0.12
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	2	0.12
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	8	0.12
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	8	0.12
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	8	0.12
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	2	0.12
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	4	0.12
(1,2266)	1:75:A:ALA:HA	1:77:A:LEU:H	7	0.12
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	3	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	3	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	3	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	3	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	5	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	5	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	5	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	6	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	6	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	6	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	7	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	7	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	7	0.12
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	10	0.12
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	10	0.12
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	10	0.12
(1,2196)	1:71:A:GLU:HA	1:75:A:ALA:H	2	0.12
(1,2162)	1:68:A:LEU:HD21	1:68:A:LEU:H	1	0.12
(1,2162)	1:68:A:LEU:HD22	1:68:A:LEU:H	1	0.12
(1,2162)	1:68:A:LEU:HD23	1:68:A:LEU:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:68:A:LEU:HB3	1:68:A:LEU:H	6	0.12
(1,2131)	1:63:A:LYS:H	1:64:A:ARG:HG3	10	0.12
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	6	0.12
(1,2084)	1:57:A:LEU:HG	1:57:A:LEU:H	2	0.12
(1,2080)	1:56:A:HIS:HA	1:58:A:VAL:H	6	0.12
(1,2071)	1:55:A:LEU:H	1:57:A:LEU:H	1	0.12
(1,2059)	1:54:A:ALA:HA	1:56:A:HIS:H	6	0.12
(1,2042)	1:52:A:LEU:HB2	1:54:A:ALA:H	3	0.12
(1,2028)	1:51:A:ASN:H	1:53:A:LEU:H	3	0.12
(1,2026)	1:51:A:ASN:HB3	1:53:A:LEU:H	2	0.12
(1,2011)	1:51:A:ASN:HA	1:51:A:ASN:HD21	4	0.12
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	8	0.12
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	8	0.12
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	8	0.12
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	9	0.12
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	9	0.12
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	9	0.12
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	10	0.12
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	10	0.12
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	10	0.12
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	4	0.12
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	4	0.12
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	4	0.12
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	9	0.12
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	9	0.12
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	9	0.12
(1,1888)	1:44:A:VAL:HG11	1:44:A:VAL:H	10	0.12
(1,1888)	1:44:A:VAL:HG12	1:44:A:VAL:H	10	0.12
(1,1888)	1:44:A:VAL:HG13	1:44:A:VAL:H	10	0.12
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	1	0.12
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	3	0.12
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	2	0.12
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	4	0.12
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	2	0.12
(1,1655)	1:32:A:ILE:HG12	1:32:A:ILE:H	6	0.12
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	1	0.12
(1,1560)	1:27:A:TRP:HA	1:28:A:GLN:HE22	10	0.12
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	5	0.12
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	2	0.12
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	2	0.12
(1,1532)	1:26:A:ARG:HB2	1:27:A:TRP:H	4	0.12
(1,1532)	1:26:A:ARG:HB3	1:27:A:TRP:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:26:A:ARG:HD2	1:27:A:TRP:H	5	0.12
(1,1523)	1:26:A:ARG:HG2	1:26:A:ARG:H	4	0.12
(1,1523)	1:26:A:ARG:HG3	1:26:A:ARG:H	4	0.12
(1,1505)	1:25:A:LEU:HG	1:26:A:ARG:H	6	0.12
(1,1493)	1:24:A:ASP:HA	1:25:A:LEU:H	2	0.12
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG21	1	0.12
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG22	1	0.12
(1,1485)	1:23:A:GLN:HE21	1:85:A:ILE:HG23	1	0.12
(1,1464)	1:22:A:ASP:HB2	1:25:A:LEU:H	8	0.12
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	4	0.12
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	5	0.12
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	7	0.12
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	1	0.12
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	1	0.12
(1,1385)	1:17:A:GLU:H	1:20:A:THR:HA	1	0.12
(1,1349)	1:15:A:THR:HB	1:27:A:TRP:HE1	9	0.12
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	2	0.12
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	2	0.12
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	2	0.12
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	6	0.12
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	6	0.12
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	6	0.12
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	9	0.12
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	9	0.12
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	9	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	2	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	2	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	4	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	4	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	6	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	6	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	9	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	9	0.12
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	10	0.12
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	10	0.12
(1,1218)	1:9:A:ARG:HB2	1:11:A:VAL:H	6	0.12
(1,1218)	1:9:A:ARG:HB2	1:11:A:VAL:H	9	0.12
(1,1216)	1:9:A:ARG:H	1:11:A:VAL:H	5	0.12
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	1	0.12
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	1	0.12
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	7	0.12
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD1	1	0.12
(1,1156)	1:119:A:PHE:HB3	1:119:A:PHE:HD2	1	0.12
(1,1152)	1:117:A:TYR:HB2	1:119:A:PHE:HB3	4	0.12
(1,1116)	1:114:A:ARG:HB3	1:114:A:ARG:HD3	6	0.12
(1,1081)	1:110:A:LYS:HA	1:110:A:LYS:HG3	5	0.12
(1,1070)	1:109:A:LEU:HA	1:112:A:GLN:HB2	3	0.12
(1,1056)	1:108:A:ALA:HB1	1:111:A:ARG:HB2	2	0.12
(1,1056)	1:108:A:ALA:HB2	1:111:A:ARG:HB2	2	0.12
(1,1056)	1:108:A:ALA:HB3	1:111:A:ARG:HB2	2	0.12
(1,1056)	1:108:A:ALA:HB1	1:111:A:ARG:HB2	9	0.12
(1,1056)	1:108:A:ALA:HB2	1:111:A:ARG:HB2	9	0.12
(1,1056)	1:108:A:ALA:HB3	1:111:A:ARG:HB2	9	0.12
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD11	9	0.12
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD12	9	0.12
(1,1023)	1:105:A:VAL:HG11	1:109:A:LEU:HD13	9	0.12
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD11	9	0.12
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD12	9	0.12
(1,1023)	1:105:A:VAL:HG12	1:109:A:LEU:HD13	9	0.12
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD11	9	0.12
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD12	9	0.12
(1,1023)	1:105:A:VAL:HG13	1:109:A:LEU:HD13	9	0.12
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	3	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	3	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	3	0.12
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	4	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	4	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	4	0.12
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	7	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	7	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	7	0.12
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	8	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	8	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	8	0.12
(1,993)	1:103:A:LEU:HD11	1:103:A:LEU:HB2	9	0.12
(1,993)	1:103:A:LEU:HD12	1:103:A:LEU:HB2	9	0.12
(1,993)	1:103:A:LEU:HD13	1:103:A:LEU:HB2	9	0.12
(1,991)	1:103:A:LEU:HD11	1:103:A:LEU:HA	2	0.12
(1,991)	1:103:A:LEU:HD12	1:103:A:LEU:HA	2	0.12
(1,991)	1:103:A:LEU:HD13	1:103:A:LEU:HA	2	0.12
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	1	0.12
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	4	0.12
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	7	0.12
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	7	0.12
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	7	0.12
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	7	0.12
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	7	0.12
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	8	0.12
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	8	0.12
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	9	0.12
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	9	0.12
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	5	0.12
(1,932)	1:93:A:GLU:HA	1:96:A:LYS:HA	4	0.12
(1,932)	1:93:A:GLU:HA	1:96:A:LYS:HA	8	0.12
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	4	0.12
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	4	0.12
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	4	0.12
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	1	0.12
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	1	0.12
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	1	0.12
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD2	7	0.12
(1,703)	1:74:A:ARG:HB2	1:74:A:ARG:HD3	7	0.12
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD11	2	0.12
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD12	2	0.12
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD13	2	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD11	2	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD12	2	0.12
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD13	2	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD11	2	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD12	2	0.12
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD13	2	0.12
(1,666)	1:71:A:GLU:HA	1:71:A:GLU:HG2	3	0.12
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG11	9	0.12
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG12	9	0.12
(1,661)	1:70:A:TYR:HD2	1:73:A:VAL:HG13	9	0.12
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	3	0.12
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	3	0.12
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD2	6	0.12
(1,603)	1:60:A:ARG:HB3	1:60:A:ARG:HD3	6	0.12
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	10	0.12
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	10	0.12
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	10	0.12
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	7	0.12
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	10	0.12
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	10	0.12
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	10	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	4	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	4	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	4	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	4	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	4	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	4	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	4	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	4	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	4	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	10	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	10	0.12
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	10	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	10	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	10	0.12
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	10	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	10	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	10	0.12
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	10	0.12
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	7	0.12
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	7	0.12
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	10	0.12
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	10	0.12
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	3	0.12
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	8	0.12
(1,364)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	1	0.12
(1,364)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	1	0.12
(1,364)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	1	0.12
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	1	0.12
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	1	0.12
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	1	0.12
(1,355)	1:34:A:ALA:HB1	1:105:A:VAL:HB	9	0.12
(1,355)	1:34:A:ALA:HB2	1:105:A:VAL:HB	9	0.12
(1,355)	1:34:A:ALA:HB3	1:105:A:VAL:HB	9	0.12
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	4	0.12
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	4	0.12
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	4	0.12
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	7	0.12
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	7	0.12
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	8	0.12
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	8	0.12
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	8	0.12
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	10	0.12
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	10	0.12
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	10	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	4	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	4	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	4	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	4	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	4	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	4	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	4	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	4	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	4	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	7	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	7	0.12
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	7	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	7	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	7	0.12
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	7	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	7	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	7	0.12
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	7	0.12
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	2	0.12
(1,309)	1:30:A:MET:HB2	1:103:A:LEU:HB2	9	0.12
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	1	0.12
(1,305)	1:30:A:MET:HA	1:33:A:MET:HB3	10	0.12
(1,301)	1:30:A:MET:HG2	1:30:A:MET:HA	4	0.12
(1,284)	1:28:A:GLN:HG2	1:99:A:THR:HA	5	0.12
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	2	0.12
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	2	0.12
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	2	0.12
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	2	0.12
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	5	0.12
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	7	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	1	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	1	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	1	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	3	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	3	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	4	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	4	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	4	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	5	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	5	0.12
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	5	0.12
(1,193)	1:25:A:LEU:HG	1:25:A:LEU:HA	5	0.12
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	5	0.12
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	6	0.12
(1,165)	1:21:A:LYS:HD2	1:21:A:LYS:HA	2	0.12
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	2	0.12
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	2	0.12
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	2	0.12
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	7	0.12
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	7	0.12
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	7	0.12
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	9	0.12
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	9	0.12
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	9	0.12
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	10	0.12
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	10	0.12
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	10	0.12
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD21	3	0.12
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD22	3	0.12
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD23	3	0.12
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD21	3	0.12
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD22	3	0.12
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD23	3	0.12
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	4	0.12
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	3	0.12
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	3	0.12
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	3	0.12
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	3	0.12
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	3	0.12
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	1	0.12
(1,60)	1:10:A:LEU:HA	1:13:A:GLU:HB2	5	0.12
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD11	7	0.12
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD12	7	0.12
(1,14)	1:5:A:ILE:HB	1:5:A:ILE:HD13	7	0.12
(1,10)	1:4:A:LYS:HG3	1:4:A:LYS:HA	5	0.12
(2,98)	1:87:A:ASP:O	1:91:A:TYR:N	9	0.11
(2,95)	1:86:A:ARG:O	1:90:A:THR:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	2	0.11
(2,46)	1:39:A:SER:O	1:43:A:LEU:N	8	0.11
(2,40)	1:36:A:GLN:O	1:40:A:GLU:N	3	0.11
(2,30)	1:31:A:ALA:O	1:35:A:LEU:N	4	0.11
(2,29)	1:31:A:ALA:O	1:35:A:LEU:H	1	0.11
(2,23)	1:16:A:ASP:O	1:20:A:THR:H	8	0.11
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	1	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	1	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	1	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	1	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG21	8	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG22	8	0.11
(1,3192)	1:80:A:PHE:HZ	1:84:A:VAL:HG23	8	0.11
(1,3166)	1:38:A:ALA:HA	1:80:A:PHE:HZ	9	0.11
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	5	0.11
(1,3133)	1:16:A:ASP:HB3	1:27:A:TRP:HZ2	10	0.11
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	6	0.11
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	8	0.11
(1,3099)	1:117:A:TYR:HB3	1:118:A:GLY:H	7	0.11
(1,3081)	1:116:A:LEU:HB2	1:116:A:LEU:H	2	0.11
(1,3077)	1:115:A:THR:HB	1:116:A:LEU:H	1	0.11
(1,3075)	1:115:A:THR:HG21	1:116:A:LEU:H	2	0.11
(1,3075)	1:115:A:THR:HG22	1:116:A:LEU:H	2	0.11
(1,3075)	1:115:A:THR:HG23	1:116:A:LEU:H	2	0.11
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	2	0.11
(1,3070)	1:114:A:ARG:HB2	1:115:A:THR:H	4	0.11
(1,3064)	1:114:A:ARG:H	1:115:A:THR:HA	9	0.11
(1,3053)	1:113:A:GLY:H	1:114:A:ARG:HA	6	0.11
(1,3031)	1:111:A:ARG:H	1:114:A:ARG:H	6	0.11
(1,3025)	1:111:A:ARG:H	1:112:A:GLN:HB2	9	0.11
(1,2969)	1:109:A:LEU:HD11	1:109:A:LEU:H	9	0.11
(1,2969)	1:109:A:LEU:HD12	1:109:A:LEU:H	9	0.11
(1,2969)	1:109:A:LEU:HD13	1:109:A:LEU:H	9	0.11
(1,2950)	1:107:A:TYR:H	1:110:A:LYS:HB2	1	0.11
(1,2927)	1:106:A:VAL:HA	1:109:A:LEU:H	3	0.11
(1,2867)	1:104:A:ASP:HB2	1:105:A:VAL:H	5	0.11
(1,2831)	1:102:A:SER:HA	1:105:A:VAL:H	9	0.11
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	3	0.11
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	3	0.11
(1,2766)	1:98:A:LYS:HG2	1:98:A:LYS:H	6	0.11
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	1	0.11
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	5	0.11
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	9	0.11
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	10	0.11
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	1	0.11
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	2	0.11
(1,2703)	1:93:A:GLU:HA	1:98:A:LYS:H	2	0.11
(1,2703)	1:93:A:GLU:HA	1:98:A:LYS:H	3	0.11
(1,2702)	1:93:A:GLU:HA	1:97:A:ARG:H	5	0.11
(1,2702)	1:93:A:GLU:HA	1:97:A:ARG:H	6	0.11
(1,2702)	1:93:A:GLU:HA	1:97:A:ARG:H	7	0.11
(1,2671)	1:92:A:THR:HA	1:97:A:ARG:HE	10	0.11
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	1	0.11
(1,2640)	1:91:A:TYR:HB3	1:104:A:ASP:H	9	0.11
(1,2626)	1:91:A:TYR:H	1:93:A:GLU:HB3	4	0.11
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	1	0.11
(1,2609)	1:90:A:THR:HA	1:93:A:GLU:H	10	0.11
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	5	0.11
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	5	0.11
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	5	0.11
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	6	0.11
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	6	0.11
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	6	0.11
(1,2577)	1:89:A:VAL:HG11	1:89:A:VAL:H	7	0.11
(1,2577)	1:89:A:VAL:HG12	1:89:A:VAL:H	7	0.11
(1,2577)	1:89:A:VAL:HG13	1:89:A:VAL:H	7	0.11
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	1	0.11
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	3	0.11
(1,2484)	1:84:A:VAL:HA	1:112:A:GLN:HE21	6	0.11
(1,2484)	1:84:A:VAL:HA	1:112:A:GLN:HE21	8	0.11
(1,2454)	1:83:A:SER:H	1:86:A:ARG:HB2	5	0.11
(1,2445)	1:83:A:SER:HB2	1:84:A:VAL:H	4	0.11
(1,2328)	1:78:A:LYS:H	1:81:A:LEU:H	6	0.11
(1,2271)	1:76:A:VAL:HG21	1:76:A:VAL:H	7	0.11
(1,2271)	1:76:A:VAL:HG22	1:76:A:VAL:H	7	0.11
(1,2271)	1:76:A:VAL:HG23	1:76:A:VAL:H	7	0.11
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	5	0.11
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	4	0.11
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	4	0.11
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	4	0.11
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	9	0.11
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	9	0.11
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:68:A:LEU:HA	1:69:A:ILE:H	5	0.11
(1,2157)	1:67:A:GLY:H	1:68:A:LEU:H	9	0.11
(1,2152)	1:65:A:ILE:H	1:66:A:SER:HA	10	0.11
(1,2147)	1:65:A:ILE:HA	1:66:A:SER:H	1	0.11
(1,2142)	1:65:A:ILE:HG13	1:65:A:ILE:H	7	0.11
(1,2106)	1:60:A:ARG:HG2	1:60:A:ARG:H	9	0.11
(1,2106)	1:60:A:ARG:HG3	1:60:A:ARG:H	9	0.11
(1,2093)	1:58:A:VAL:HB	1:58:A:VAL:H	6	0.11
(1,2075)	1:56:A:HIS:H	1:57:A:LEU:H	1	0.11
(1,2042)	1:52:A:LEU:HB2	1:54:A:ALA:H	7	0.11
(1,2028)	1:51:A:ASN:H	1:53:A:LEU:H	6	0.11
(1,2017)	1:51:A:ASN:HD22	1:52:A:LEU:HD21	7	0.11
(1,2017)	1:51:A:ASN:HD22	1:52:A:LEU:HD22	7	0.11
(1,2017)	1:51:A:ASN:HD22	1:52:A:LEU:HD23	7	0.11
(1,1981)	1:48:A:GLU:H	1:50:A:THR:HB	9	0.11
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG21	4	0.11
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG22	4	0.11
(1,1941)	1:46:A:LEU:H	1:50:A:THR:HG23	4	0.11
(1,1932)	1:46:A:LEU:HB2	1:47:A:LEU:H	2	0.11
(1,1932)	1:46:A:LEU:HB2	1:47:A:LEU:H	5	0.11
(1,1932)	1:46:A:LEU:HB2	1:47:A:LEU:H	9	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	1	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	1	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	1	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	2	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	2	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	2	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	3	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	3	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	3	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	4	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	4	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	4	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	6	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	6	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	6	0.11
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	7	0.11
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	7	0.11
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	7	0.11
(1,1900)	1:44:A:VAL:HG21	1:46:A:LEU:H	10	0.11
(1,1900)	1:44:A:VAL:HG22	1:46:A:LEU:H	10	0.11
(1,1900)	1:44:A:VAL:HG23	1:46:A:LEU:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	2	0.11
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	4	0.11
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	6	0.11
(1,1883)	1:43:A:LEU:HG	1:46:A:LEU:H	7	0.11
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	1	0.11
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	9	0.11
(1,1788)	1:38:A:ALA:HA	1:41:A:ALA:H	10	0.11
(1,1760)	1:36:A:GLN:HE21	1:39:A:SER:H	6	0.11
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	1	0.11
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	2	0.11
(1,1730)	1:35:A:LEU:HB2	1:37:A:GLU:H	1	0.11
(1,1707)	1:34:A:ALA:H	1:36:A:GLN:H	2	0.11
(1,1643)	1:31:A:ALA:H	1:100:A:VAL:HB	6	0.11
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	5	0.11
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	9	0.11
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	10	0.11
(1,1592)	1:28:A:GLN:H	1:99:A:THR:HA	8	0.11
(1,1541)	1:26:A:ARG:HD2	1:98:A:LYS:H	9	0.11
(1,1536)	1:26:A:ARG:HG2	1:28:A:GLN:H	6	0.11
(1,1536)	1:26:A:ARG:HG3	1:28:A:GLN:H	6	0.11
(1,1530)	1:26:A:ARG:HD2	1:27:A:TRP:H	2	0.11
(1,1480)	1:23:A:GLN:HG2	1:24:A:ASP:H	4	0.11
(1,1450)	1:22:A:ASP:H	1:23:A:GLN:H	6	0.11
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	3	0.11
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	7	0.11
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	10	0.11
(1,1372)	1:17:A:GLU:HG2	1:17:A:GLU:H	7	0.11
(1,1372)	1:17:A:GLU:HG2	1:17:A:GLU:H	10	0.11
(1,1333)	1:15:A:THR:HG21	1:15:A:THR:H	1	0.11
(1,1333)	1:15:A:THR:HG22	1:15:A:THR:H	1	0.11
(1,1333)	1:15:A:THR:HG23	1:15:A:THR:H	1	0.11
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	3	0.11
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	3	0.11
(1,1246)	1:11:A:VAL:HG21	1:11:A:VAL:H	1	0.11
(1,1246)	1:11:A:VAL:HG22	1:11:A:VAL:H	1	0.11
(1,1246)	1:11:A:VAL:HG23	1:11:A:VAL:H	1	0.11
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	4	0.11
(1,1158)	1:120:A:GLY:HA2	1:121:A:GLY:HA3	3	0.11
(1,1132)	1:116:A:LEU:HD21	1:116:A:LEU:HB2	2	0.11
(1,1132)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	2	0.11
(1,1132)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	2	0.11
(1,1132)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:116:A:LEU:HD23	1:116:A:LEU:HB2	2	0.11
(1,1132)	1:116:A:LEU:HD23	1:116:A:LEU:HB3	2	0.11
(1,1092)	1:110:A:LYS:HB3	1:111:A:ARG:HB3	6	0.11
(1,1056)	1:108:A:ALA:HB1	1:111:A:ARG:HB2	3	0.11
(1,1056)	1:108:A:ALA:HB2	1:111:A:ARG:HB2	3	0.11
(1,1056)	1:108:A:ALA:HB3	1:111:A:ARG:HB2	3	0.11
(1,1056)	1:108:A:ALA:HB1	1:111:A:ARG:HB2	5	0.11
(1,1056)	1:108:A:ALA:HB2	1:111:A:ARG:HB2	5	0.11
(1,1056)	1:108:A:ALA:HB3	1:111:A:ARG:HB2	5	0.11
(1,1019)	1:105:A:VAL:HA	1:107:A:TYR:HA	4	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	3	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	3	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	3	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	8	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	8	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	8	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	10	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	10	0.11
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	10	0.11
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG21	9	0.11
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG22	9	0.11
(1,958)	1:97:A:ARG:HG2	1:101:A:THR:HG23	9	0.11
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG21	9	0.11
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG22	9	0.11
(1,958)	1:97:A:ARG:HG3	1:101:A:THR:HG23	9	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	3	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	3	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	5	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	5	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD2	6	0.11
(1,955)	1:97:A:ARG:HB2	1:97:A:ARG:HD3	6	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD2	5	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD3	5	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD2	5	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD3	5	0.11
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD2	5	0.11
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD3	5	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD2	6	0.11
(1,939)	1:95:A:ALA:HB1	1:97:A:ARG:HD3	6	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD2	6	0.11
(1,939)	1:95:A:ALA:HB2	1:97:A:ARG:HD3	6	0.11
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:95:A:ALA:HB3	1:97:A:ARG:HD3	6	0.11
(1,932)	1:93:A:GLU:HA	1:96:A:LYS:HA	10	0.11
(1,918)	1:92:A:THR:HG21	1:98:A:LYS:HA	5	0.11
(1,918)	1:92:A:THR:HG22	1:98:A:LYS:HA	5	0.11
(1,918)	1:92:A:THR:HG23	1:98:A:LYS:HA	5	0.11
(1,868)	1:87:A:ASP:HB3	1:104:A:ASP:HB3	2	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	2	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	2	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	2	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	3	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	3	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	3	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	10	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	10	0.11
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	10	0.11
(1,743)	1:77:A:LEU:HD11	1:80:A:PHE:HE2	4	0.11
(1,743)	1:77:A:LEU:HD12	1:80:A:PHE:HE2	4	0.11
(1,743)	1:77:A:LEU:HD13	1:80:A:PHE:HE2	4	0.11
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD11	3	0.11
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD12	3	0.11
(1,696)	1:73:A:VAL:HG11	1:77:A:LEU:HD13	3	0.11
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD11	3	0.11
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD12	3	0.11
(1,696)	1:73:A:VAL:HG12	1:77:A:LEU:HD13	3	0.11
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD11	3	0.11
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD12	3	0.11
(1,696)	1:73:A:VAL:HG13	1:77:A:LEU:HD13	3	0.11
(1,690)	1:73:A:VAL:HB	1:76:A:VAL:HG11	1	0.11
(1,690)	1:73:A:VAL:HB	1:76:A:VAL:HG12	1	0.11
(1,690)	1:73:A:VAL:HB	1:76:A:VAL:HG13	1	0.11
(1,657)	1:70:A:TYR:HB3	1:70:A:TYR:HD1	9	0.11
(1,657)	1:70:A:TYR:HB3	1:70:A:TYR:HD2	9	0.11
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB2	10	0.11
(1,645)	1:68:A:LEU:HB3	1:71:A:GLU:HB3	10	0.11
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD2	2	0.11
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD3	2	0.11
(1,616)	1:63:A:LYS:HG2	1:65:A:ILE:HG12	5	0.11
(1,546)	1:53:A:LEU:HD21	1:57:A:LEU:HB2	9	0.11
(1,546)	1:53:A:LEU:HD22	1:57:A:LEU:HB2	9	0.11
(1,546)	1:53:A:LEU:HD23	1:57:A:LEU:HB2	9	0.11
(1,545)	1:53:A:LEU:HA	1:57:A:LEU:HB3	6	0.11
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG22	3	0.11
(1,515)	1:47:A:LEU:HA	1:50:A:THR:HG23	3	0.11
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	4	0.11
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD11	9	0.11
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD12	9	0.11
(1,449)	1:43:A:LEU:HA	1:46:A:LEU:HD13	9	0.11
(1,444)	1:43:A:LEU:HA	1:46:A:LEU:HB3	2	0.11
(1,444)	1:43:A:LEU:HA	1:46:A:LEU:HB3	10	0.11
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	2	0.11
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	2	0.11
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	2	0.11
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	2	0.11
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	2	0.11
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	2	0.11
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	2	0.11
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	2	0.11
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	2	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	2	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	2	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	4	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	4	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	5	0.11
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	5	0.11
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD11	4	0.11
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD12	4	0.11
(1,399)	1:40:A:GLU:HA	1:43:A:LEU:HD13	4	0.11
(1,369)	1:35:A:LEU:HA	1:37:A:GLU:HB2	9	0.11
(1,363)	1:35:A:LEU:HD21	1:35:A:LEU:HB3	4	0.11
(1,363)	1:35:A:LEU:HD22	1:35:A:LEU:HB3	4	0.11
(1,363)	1:35:A:LEU:HD23	1:35:A:LEU:HB3	4	0.11
(1,360)	1:35:A:LEU:HA	1:35:A:LEU:HG	7	0.11
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB2	10	0.11
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB3	10	0.11
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB2	10	0.11
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB3	10	0.11
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB2	10	0.11
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB3	10	0.11
(1,347)	1:34:A:ALA:HA	1:37:A:GLU:HB2	2	0.11
(1,347)	1:34:A:ALA:HA	1:37:A:GLU:HB3	2	0.11
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	2	0.11
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	2	0.11
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	9	0.11
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	9	0.11
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	9	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	9	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	9	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	9	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	9	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	9	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	9	0.11
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG11	10	0.11
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG12	10	0.11
(1,318)	1:31:A:ALA:HB1	1:100:A:VAL:HG13	10	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG11	10	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG12	10	0.11
(1,318)	1:31:A:ALA:HB2	1:100:A:VAL:HG13	10	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG11	10	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG12	10	0.11
(1,318)	1:31:A:ALA:HB3	1:100:A:VAL:HG13	10	0.11
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG21	10	0.11
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG22	10	0.11
(1,283)	1:28:A:GLN:HG2	1:99:A:THR:HG23	10	0.11
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	4	0.11
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	10	0.11
(1,238)	1:26:A:ARG:HA	1:99:A:THR:HA	9	0.11
(1,232)	1:26:A:ARG:HA	1:26:A:ARG:HE	4	0.11
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	7	0.11
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	7	0.11
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	7	0.11
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	7	0.11
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	7	0.11
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	7	0.11
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	7	0.11
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	7	0.11
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	7	0.11
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG21	4	0.11
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG22	4	0.11
(1,204)	1:25:A:LEU:HD21	1:89:A:VAL:HG23	4	0.11
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG21	4	0.11
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG22	4	0.11
(1,204)	1:25:A:LEU:HD22	1:89:A:VAL:HG23	4	0.11
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG21	4	0.11
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:25:A:LEU:HD23	1:89:A:VAL:HG23	4	0.11
(1,201)	1:25:A:LEU:HD11	1:27:A:TRP:HD1	9	0.11
(1,201)	1:25:A:LEU:HD12	1:27:A:TRP:HD1	9	0.11
(1,201)	1:25:A:LEU:HD13	1:27:A:TRP:HD1	9	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	6	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	6	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	6	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	7	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	7	0.11
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	7	0.11
(1,187)	1:23:A:GLN:HG2	1:25:A:LEU:HD11	8	0.11
(1,187)	1:23:A:GLN:HG2	1:25:A:LEU:HD12	8	0.11
(1,187)	1:23:A:GLN:HG2	1:25:A:LEU:HD13	8	0.11
(1,173)	1:21:A:LYS:HD2	1:86:A:ARG:HG2	7	0.11
(1,172)	1:21:A:LYS:HD2	1:85:A:ILE:HG12	4	0.11
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD11	5	0.11
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD12	5	0.11
(1,170)	1:21:A:LYS:HB3	1:25:A:LEU:HD13	5	0.11
(1,165)	1:21:A:LYS:HD2	1:21:A:LYS:HA	8	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD21	4	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD22	4	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD23	4	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD21	4	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD22	4	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD23	4	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD21	4	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD22	4	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD23	4	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD21	8	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD22	8	0.11
(1,131)	1:15:A:THR:HG21	1:35:A:LEU:HD23	8	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD21	8	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD22	8	0.11
(1,131)	1:15:A:THR:HG22	1:35:A:LEU:HD23	8	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD21	8	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD22	8	0.11
(1,131)	1:15:A:THR:HG23	1:35:A:LEU:HD23	8	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD11	10	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD12	10	0.11
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD13	10	0.11
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD11	10	0.11
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD13	10	0.11
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD11	10	0.11
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD12	10	0.11
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD13	10	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD21	9	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD22	9	0.11
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD23	9	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD21	9	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD22	9	0.11
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD23	9	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD21	9	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD22	9	0.11
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD23	9	0.11
(1,112)	1:14:A:VAL:HG21	1:17:A:GLU:HB2	1	0.11
(1,112)	1:14:A:VAL:HG22	1:17:A:GLU:HB2	1	0.11
(1,112)	1:14:A:VAL:HG23	1:17:A:GLU:HB2	1	0.11
(1,108)	1:14:A:VAL:HG21	1:15:A:THR:HA	4	0.11
(1,108)	1:14:A:VAL:HG22	1:15:A:THR:HA	4	0.11
(1,108)	1:14:A:VAL:HG23	1:15:A:THR:HA	4	0.11
(1,96)	1:12:A:LYS:HD3	1:35:A:LEU:HG	9	0.11
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	6	0.11
(1,87)	1:12:A:LYS:HD2	1:29:A:SER:HA	9	0.11
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	2	0.11
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	2	0.11
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	8	0.11
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	8	0.11
(1,85)	1:12:A:LYS:HA	1:16:A:ASP:HA	10	0.11
(1,71)	1:11:A:VAL:HG11	1:35:A:LEU:HG	2	0.11
(1,71)	1:11:A:VAL:HG12	1:35:A:LEU:HG	2	0.11
(1,71)	1:11:A:VAL:HG13	1:35:A:LEU:HG	2	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG11	5	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG12	5	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG13	5	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG11	6	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG12	6	0.11
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG13	6	0.11
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	5	0.11
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	5	0.11
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	5	0.11
(1,64)	1:11:A:VAL:HG21	1:11:A:VAL:HA	10	0.11
(1,64)	1:11:A:VAL:HG22	1:11:A:VAL:HA	10	0.11
(1,64)	1:11:A:VAL:HG23	1:11:A:VAL:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:8:A:ALA:HA	1:32:A:ILE:HG12	9	0.11
(1,13)	1:4:A:LYS:HB3	1:9:A:ARG:HD2	3	0.11
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	6	0.11
(1,9)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	6	0.11
(2,60)	1:68:A:LEU:O	1:72:A:GLU:N	7	0.1
(1,3196)	1:80:A:PHE:HZ	1:105:A:VAL:HA	7	0.1
(1,3183)	1:42:A:TYR:HE1	1:80:A:PHE:HB2	9	0.1
(1,3183)	1:42:A:TYR:HE1	1:80:A:PHE:HB3	9	0.1
(1,3169)	1:41:A:ALA:HB1	1:80:A:PHE:HZ	2	0.1
(1,3169)	1:41:A:ALA:HB2	1:80:A:PHE:HZ	2	0.1
(1,3169)	1:41:A:ALA:HB3	1:80:A:PHE:HZ	2	0.1
(1,3130)	1:15:A:THR:HA	1:18:A:PHE:HZ	9	0.1
(1,3105)	1:118:A:GLY:HA2	1:119:A:PHE:H	10	0.1
(1,3093)	1:116:A:LEU:HG	1:119:A:PHE:H	1	0.1
(1,3093)	1:116:A:LEU:HG	1:119:A:PHE:H	8	0.1
(1,3080)	1:116:A:LEU:HG	1:116:A:LEU:H	2	0.1
(1,3072)	1:115:A:THR:HB	1:115:A:THR:H	5	0.1
(1,3006)	1:110:A:LYS:HG2	1:114:A:ARG:H	10	0.1
(1,3003)	1:110:A:LYS:H	1:113:A:GLY:H	5	0.1
(1,2950)	1:107:A:TYR:H	1:110:A:LYS:HB2	8	0.1
(1,2939)	1:107:A:TYR:HB3	1:108:A:ALA:H	3	0.1
(1,2804)	1:101:A:THR:HA	1:103:A:LEU:H	9	0.1
(1,2768)	1:98:A:LYS:HD2	1:98:A:LYS:H	10	0.1
(1,2741)	1:96:A:LYS:HB2	1:98:A:LYS:H	7	0.1
(1,2739)	1:96:A:LYS:HG2	1:97:A:ARG:H	6	0.1
(1,2734)	1:96:A:LYS:HB3	1:97:A:ARG:H	4	0.1
(1,2687)	1:93:A:GLU:HG2	1:94:A:HIS:H	5	0.1
(1,2687)	1:93:A:GLU:HG2	1:94:A:HIS:H	7	0.1
(1,2680)	1:93:A:GLU:HG2	1:93:A:GLU:H	5	0.1
(1,2680)	1:93:A:GLU:HG2	1:93:A:GLU:H	7	0.1
(1,2572)	1:88:A:SER:H	1:92:A:THR:H	7	0.1
(1,2531)	1:86:A:ARG:HA	1:88:A:SER:H	5	0.1
(1,2454)	1:83:A:SER:H	1:86:A:ARG:HB2	4	0.1
(1,2422)	1:82:A:GLU:HB2	1:83:A:SER:H	4	0.1
(1,2422)	1:82:A:GLU:HB2	1:83:A:SER:H	9	0.1
(1,2422)	1:82:A:GLU:HB2	1:83:A:SER:H	10	0.1
(1,2273)	1:76:A:VAL:HB	1:77:A:LEU:H	4	0.1
(1,2265)	1:75:A:ALA:H	1:77:A:LEU:HB2	8	0.1
(1,2209)	1:73:A:VAL:HG11	1:73:A:VAL:H	2	0.1
(1,2209)	1:73:A:VAL:HG12	1:73:A:VAL:H	2	0.1
(1,2209)	1:73:A:VAL:HG13	1:73:A:VAL:H	2	0.1
(1,2163)	1:68:A:LEU:HG	1:68:A:LEU:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:65:A:ILE:HG13	1:65:A:ILE:H	5	0.1
(1,2141)	1:65:A:ILE:HG12	1:65:A:ILE:H	4	0.1
(1,2136)	1:64:A:ARG:HA	1:65:A:ILE:H	4	0.1
(1,2136)	1:64:A:ARG:HA	1:65:A:ILE:H	7	0.1
(1,2091)	1:57:A:LEU:HB2	1:58:A:VAL:H	5	0.1
(1,2072)	1:55:A:LEU:HA	1:57:A:LEU:H	7	0.1
(1,2023)	1:51:A:ASN:HD21	1:52:A:LEU:HB3	7	0.1
(1,2019)	1:51:A:ASN:HD22	1:52:A:LEU:HB3	3	0.1
(1,2000)	1:50:A:THR:HB	1:51:A:ASN:H	5	0.1
(1,1923)	1:46:A:LEU:HD21	1:46:A:LEU:H	5	0.1
(1,1923)	1:46:A:LEU:HD22	1:46:A:LEU:H	5	0.1
(1,1923)	1:46:A:LEU:HD23	1:46:A:LEU:H	5	0.1
(1,1900)	1:44:A:VAL:HG21	1:46:A:LEU:H	7	0.1
(1,1900)	1:44:A:VAL:HG22	1:46:A:LEU:H	7	0.1
(1,1900)	1:44:A:VAL:HG23	1:46:A:LEU:H	7	0.1
(1,1846)	1:42:A:TYR:HB2	1:43:A:LEU:H	6	0.1
(1,1809)	1:40:A:GLU:HG2	1:40:A:GLU:H	3	0.1
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	5	0.1
(1,1776)	1:37:A:GLU:H	1:40:A:GLU:HB2	7	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	4	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	5	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	7	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	8	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	9	0.1
(1,1743)	1:36:A:GLN:HG3	1:36:A:GLN:HE21	10	0.1
(1,1707)	1:34:A:ALA:H	1:36:A:GLN:H	3	0.1
(1,1707)	1:34:A:ALA:H	1:36:A:GLN:H	7	0.1
(1,1628)	1:30:A:MET:HB3	1:102:A:SER:H	8	0.1
(1,1520)	1:25:A:LEU:HD11	1:99:A:THR:H	2	0.1
(1,1520)	1:25:A:LEU:HD12	1:99:A:THR:H	2	0.1
(1,1520)	1:25:A:LEU:HD13	1:99:A:THR:H	2	0.1
(1,1506)	1:25:A:LEU:HB2	1:26:A:ARG:H	8	0.1
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	5	0.1
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	5	0.1
(1,1442)	1:21:A:LYS:HG2	1:24:A:ASP:H	7	0.1
(1,1442)	1:21:A:LYS:HG3	1:24:A:ASP:H	7	0.1
(1,1427)	1:20:A:THR:HA	1:23:A:GLN:H	8	0.1
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	5	0.1
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	6	0.1
(1,1386)	1:17:A:GLU:H	1:20:A:THR:HB	8	0.1
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	5	0.1
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:12:A:LYS:HG2	1:13:A:GLU:H	7	0.1
(1,1275)	1:12:A:LYS:HG3	1:13:A:GLU:H	7	0.1
(1,1246)	1:11:A:VAL:HG21	1:11:A:VAL:H	2	0.1
(1,1246)	1:11:A:VAL:HG22	1:11:A:VAL:H	2	0.1
(1,1246)	1:11:A:VAL:HG23	1:11:A:VAL:H	2	0.1
(1,1246)	1:11:A:VAL:HG21	1:11:A:VAL:H	7	0.1
(1,1246)	1:11:A:VAL:HG22	1:11:A:VAL:H	7	0.1
(1,1246)	1:11:A:VAL:HG23	1:11:A:VAL:H	7	0.1
(1,1235)	1:10:A:LEU:H	1:12:A:LYS:HB3	10	0.1
(1,1219)	1:9:A:ARG:H	1:12:A:LYS:H	6	0.1
(1,1185)	1:7:A:PHE:HA	1:10:A:LEU:H	10	0.1
(1,1166)	1:2:A:ILE:HG21	1:3:A:SER:H	5	0.1
(1,1166)	1:2:A:ILE:HG22	1:3:A:SER:H	5	0.1
(1,1166)	1:2:A:ILE:HG23	1:3:A:SER:H	5	0.1
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB1	6	0.1
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB2	6	0.1
(1,1014)	1:104:A:ASP:HA	1:108:A:ALA:HB3	6	0.1
(1,975)	1:99:A:THR:HG21	1:101:A:THR:HG21	4	0.1
(1,975)	1:99:A:THR:HG21	1:101:A:THR:HG22	4	0.1
(1,975)	1:99:A:THR:HG21	1:101:A:THR:HG23	4	0.1
(1,975)	1:99:A:THR:HG22	1:101:A:THR:HG21	4	0.1
(1,975)	1:99:A:THR:HG22	1:101:A:THR:HG22	4	0.1
(1,975)	1:99:A:THR:HG22	1:101:A:THR:HG23	4	0.1
(1,975)	1:99:A:THR:HG23	1:101:A:THR:HG21	4	0.1
(1,975)	1:99:A:THR:HG23	1:101:A:THR:HG22	4	0.1
(1,975)	1:99:A:THR:HG23	1:101:A:THR:HG23	4	0.1
(1,960)	1:98:A:LYS:HA	1:98:A:LYS:HD3	9	0.1
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD2	7	0.1
(1,954)	1:97:A:ARG:HB3	1:97:A:ARG:HD3	7	0.1
(1,952)	1:96:A:LYS:HD2	1:97:A:ARG:HB3	9	0.1
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG21	7	0.1
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG22	7	0.1
(1,851)	1:85:A:ILE:HA	1:85:A:ILE:HG23	7	0.1
(1,658)	1:70:A:TYR:HB2	1:70:A:TYR:HD1	3	0.1
(1,658)	1:70:A:TYR:HB2	1:70:A:TYR:HD2	3	0.1
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD2	8	0.1
(1,619)	1:64:A:ARG:HB2	1:64:A:ARG:HD3	8	0.1
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	1	0.1
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	1	0.1
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	1	0.1
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	2	0.1
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	2	0.1
(1,584)	1:58:A:VAL:HG11	1:59:A:PRO:HD2	5	0.1
(1,584)	1:58:A:VAL:HG12	1:59:A:PRO:HD2	5	0.1
(1,584)	1:58:A:VAL:HG13	1:59:A:PRO:HD2	5	0.1
(1,459)	1:44:A:VAL:HA	1:47:A:LEU:HB3	5	0.1
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG21	1	0.1
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG22	1	0.1
(1,441)	1:43:A:LEU:HD11	1:44:A:VAL:HG23	1	0.1
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG21	1	0.1
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG22	1	0.1
(1,441)	1:43:A:LEU:HD12	1:44:A:VAL:HG23	1	0.1
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG21	1	0.1
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG22	1	0.1
(1,441)	1:43:A:LEU:HD13	1:44:A:VAL:HG23	1	0.1
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	1	0.1
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	1	0.1
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD1	9	0.1
(1,416)	1:42:A:TYR:HB3	1:42:A:TYR:HD2	9	0.1
(1,415)	1:42:A:TYR:HB2	1:42:A:TYR:HD1	3	0.1
(1,415)	1:42:A:TYR:HB2	1:42:A:TYR:HD2	3	0.1
(1,377)	1:36:A:GLN:HA	1:40:A:GLU:HB2	8	0.1
(1,355)	1:34:A:ALA:HB1	1:105:A:VAL:HB	6	0.1
(1,355)	1:34:A:ALA:HB2	1:105:A:VAL:HB	6	0.1
(1,355)	1:34:A:ALA:HB3	1:105:A:VAL:HB	6	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB2	8	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB3	8	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB2	8	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB3	8	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB2	8	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB3	8	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB2	9	0.1
(1,351)	1:34:A:ALA:HB1	1:102:A:SER:HB3	9	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB2	9	0.1
(1,351)	1:34:A:ALA:HB2	1:102:A:SER:HB3	9	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB2	9	0.1
(1,351)	1:34:A:ALA:HB3	1:102:A:SER:HB3	9	0.1
(1,324)	1:32:A:ILE:HD11	1:32:A:ILE:HB	1	0.1
(1,324)	1:32:A:ILE:HD12	1:32:A:ILE:HB	1	0.1
(1,324)	1:32:A:ILE:HD13	1:32:A:ILE:HB	1	0.1
(1,306)	1:30:A:MET:HA	1:33:A:MET:HG3	6	0.1
(1,290)	1:28:A:GLN:HG3	1:101:A:THR:HA	8	0.1
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD11	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD12	1	0.1
(1,256)	1:27:A:TRP:HB3	1:32:A:ILE:HD13	1	0.1
(1,247)	1:27:A:TRP:HB3	1:27:A:TRP:HE3	8	0.1
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG21	9	0.1
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG22	9	0.1
(1,224)	1:25:A:LEU:HD21	1:100:A:VAL:HG23	9	0.1
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG21	9	0.1
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG22	9	0.1
(1,224)	1:25:A:LEU:HD22	1:100:A:VAL:HG23	9	0.1
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG21	9	0.1
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG22	9	0.1
(1,224)	1:25:A:LEU:HD23	1:100:A:VAL:HG23	9	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	9	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	9	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	9	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD11	10	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD12	10	0.1
(1,197)	1:25:A:LEU:HA	1:25:A:LEU:HD13	10	0.1
(1,171)	1:21:A:LYS:HB3	1:25:A:LEU:HD21	7	0.1
(1,171)	1:21:A:LYS:HB3	1:25:A:LEU:HD22	7	0.1
(1,171)	1:21:A:LYS:HB3	1:25:A:LEU:HD23	7	0.1
(1,166)	1:21:A:LYS:HD3	1:21:A:LYS:HA	8	0.1
(1,165)	1:21:A:LYS:HD2	1:21:A:LYS:HA	3	0.1
(1,165)	1:21:A:LYS:HD2	1:21:A:LYS:HA	7	0.1
(1,138)	1:17:A:GLU:HG2	1:17:A:GLU:HA	4	0.1
(1,138)	1:17:A:GLU:HG2	1:17:A:GLU:HA	10	0.1
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD11	7	0.1
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD12	7	0.1
(1,128)	1:14:A:VAL:HG21	1:81:A:LEU:HD13	7	0.1
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD11	7	0.1
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD12	7	0.1
(1,128)	1:14:A:VAL:HG22	1:81:A:LEU:HD13	7	0.1
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD11	7	0.1
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD12	7	0.1
(1,128)	1:14:A:VAL:HG23	1:81:A:LEU:HD13	7	0.1
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD21	8	0.1
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD22	8	0.1
(1,120)	1:14:A:VAL:HG11	1:35:A:LEU:HD23	8	0.1
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD21	8	0.1
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD22	8	0.1
(1,120)	1:14:A:VAL:HG12	1:35:A:LEU:HD23	8	0.1
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD21	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD22	8	0.1
(1,120)	1:14:A:VAL:HG13	1:35:A:LEU:HD23	8	0.1
(1,100)	1:13:A:GLU:HG2	1:13:A:GLU:HA	7	0.1
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD21	10	0.1
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD22	10	0.1
(1,98)	1:12:A:LYS:HD2	1:35:A:LEU:HD23	10	0.1
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD21	10	0.1
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD22	10	0.1
(1,98)	1:12:A:LYS:HD3	1:35:A:LEU:HD23	10	0.1
(1,86)	1:12:A:LYS:HE2	1:27:A:TRP:HB3	7	0.1
(1,86)	1:12:A:LYS:HE3	1:27:A:TRP:HB3	7	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG11	3	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG12	3	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG13	3	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG11	10	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG12	10	0.1
(1,65)	1:11:A:VAL:HA	1:11:A:VAL:HG13	10	0.1
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD21	8	0.1
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD22	8	0.1
(1,53)	1:10:A:LEU:HB3	1:10:A:LEU:HD23	8	0.1
(1,40)	1:9:A:ARG:HD3	1:9:A:ARG:HB2	5	0.1

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

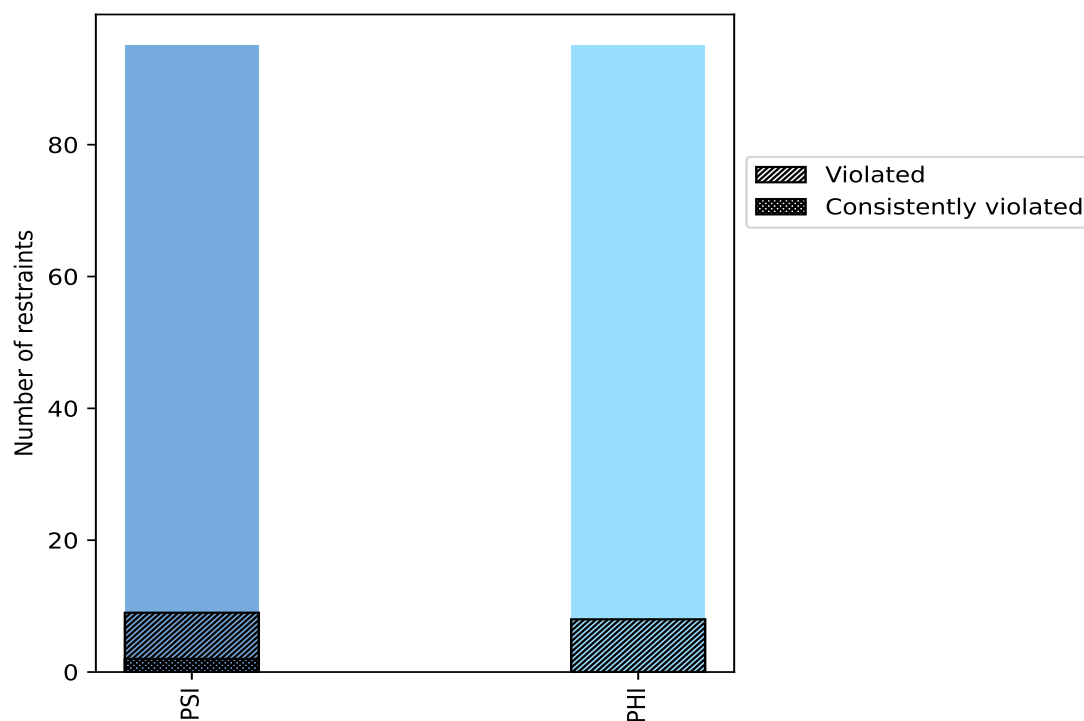
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	95	50.0	9	9.5	4.7	2	2.1	1.1
PHI	95	50.0	8	8.4	4.2	0	0.0	0.0
Total	190	100.0	17	8.9	8.9	2	1.1	1.1

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

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



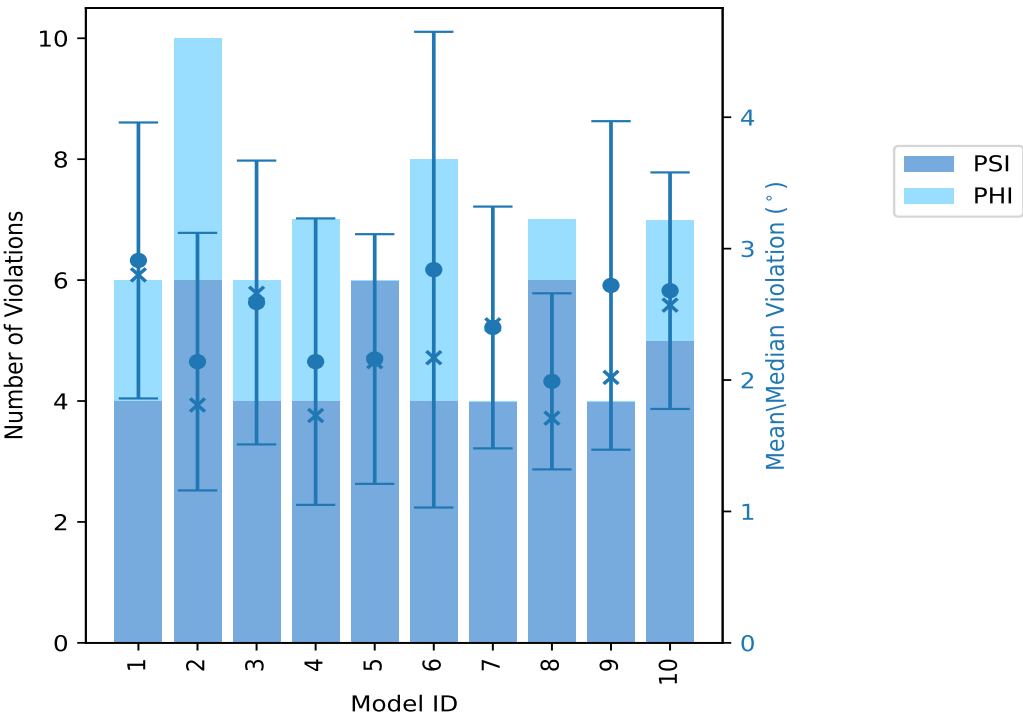
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	2	6	2.91	4.4	1.05	2.8
2	6	4	10	2.14	4.15	0.98	1.81
3	4	2	6	2.59	4.06	1.08	2.66
4	4	3	7	2.14	4.22	1.09	1.73
5	6	0	6	2.16	3.5	0.95	2.14
6	4	4	8	2.84	7.04	1.81	2.17
7	4	0	4	2.4	3.57	0.92	2.42
8	6	1	7	1.99	3.19	0.67	1.71
9	4	0	4	2.72	4.89	1.25	2.02
10	5	2	7	2.68	4.04	0.9	2.57

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

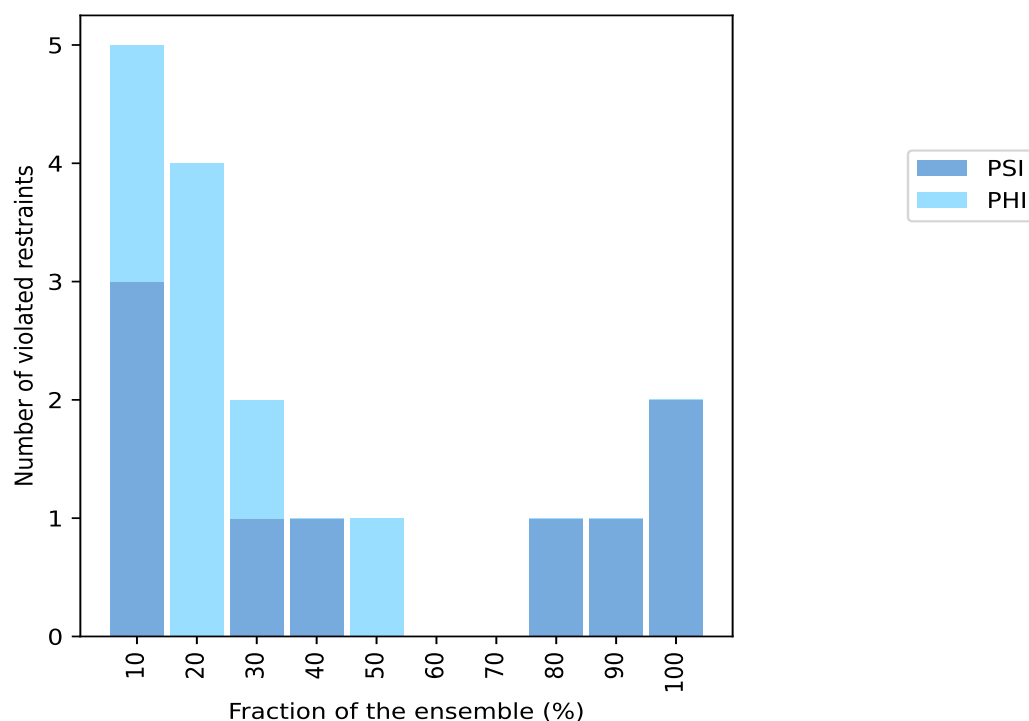
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

¹ Number of models with violations

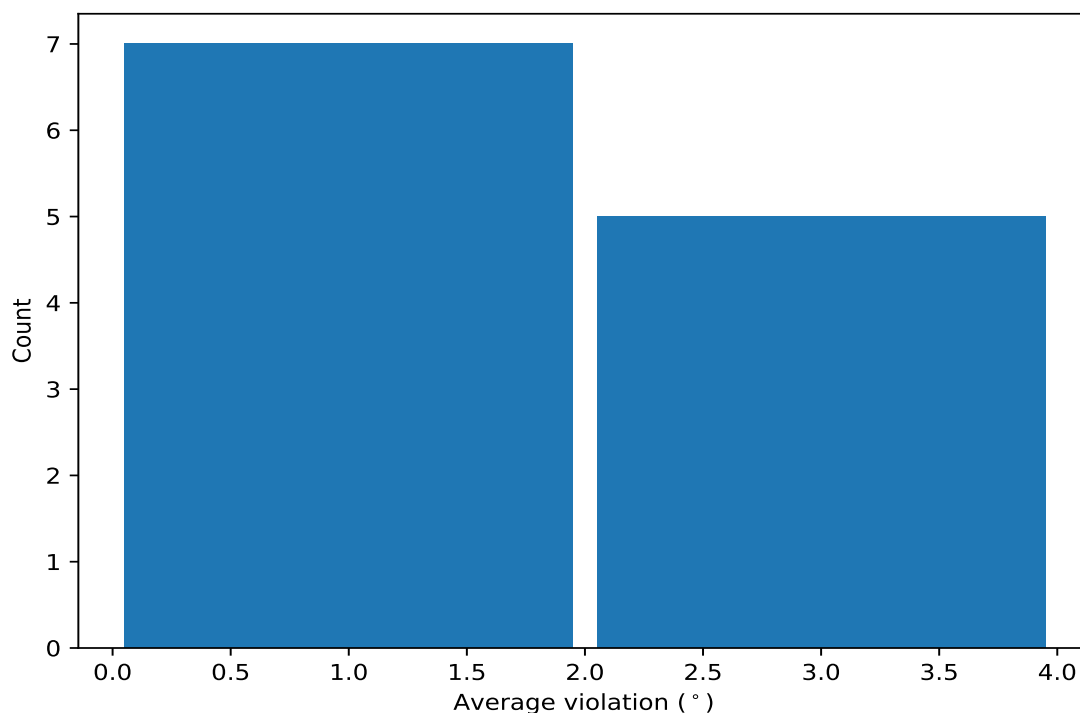
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

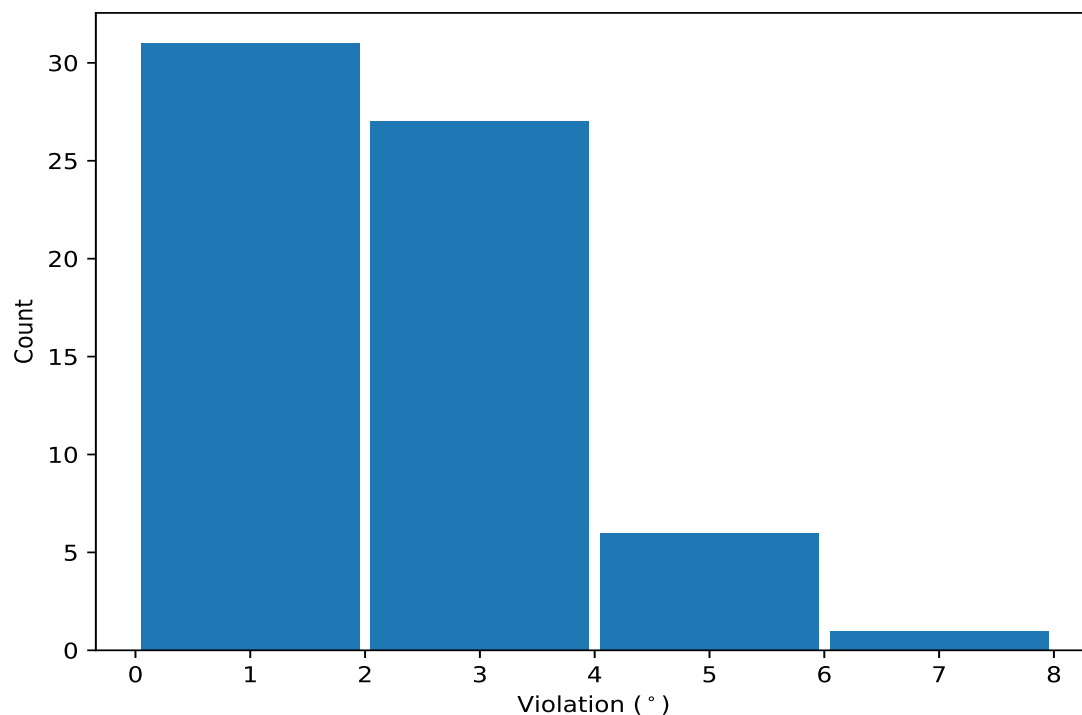
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	10	3.27	0.79	3.32
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	10	2.99	0.79	3.45
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	9	3.1	1.79	2.5
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	8	1.86	0.43	1.78
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	5	2.92	1.08	3.3
(1,178)	1:101:A:THR:N	1:101:A:THR:CA	1:101:A:THR:C	1:102:A:SER:N	4	1.47	0.38	1.42
(1,43)	1:48:A:GLU:C	1:49:A:HIS:N	1:49:A:HIS:CA	1:49:A:HIS:C	3	2.29	0.63	1.87
(1,112)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:ASP:N	3	1.91	0.62	2.07
(1,18)	1:22:A:ASP:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	2	1.52	0.06	1.52
(1,81)	1:98:A:LYS:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	2	1.25	0.05	1.25
(1,95)	1:112:A:GLN:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	2	1.18	0.12	1.18
(1,15)	1:18:A:PHE:C	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	2	1.15	0.03	1.15

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	6	7.04
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	9	4.89
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1	4.4
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	4	4.22
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	2	4.15
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	3	4.06
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	10	4.04
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	1	3.85
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	2	3.72
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	6	3.61
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	6	3.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	7	3.57
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	3	3.55
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	5	3.5
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	10	3.45
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	10	3.4
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	4	3.3
(1,145)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:ARG:N	8	3.19
(1,43)	1:48:A:GLU:C	1:49:A:HIS:N	1:49:A:HIS:CA	1:49:A:HIS:C	3	3.19
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	1	3.13
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	5	3.04
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	7	2.96
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	5	2.62
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	8	2.62
(1,112)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:ASP:N	10	2.57
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	2	2.5
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	1	2.47
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	6	2.47
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	1	2.43
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	10	2.21
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	8	2.16
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	3	2.14
(1,112)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:ASP:N	2	2.07
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	9	2.06
(1,178)	1:101:A:THR:N	1:101:A:THR:CA	1:101:A:THR:C	1:102:A:SER:N	9	1.99
(1,136)	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	1:48:A:GLU:N	9	1.95
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	7	1.89
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	4	1.89
(1,43)	1:48:A:GLU:C	1:49:A:HIS:N	1:49:A:HIS:CA	1:49:A:HIS:C	6	1.87
(1,43)	1:48:A:GLU:C	1:49:A:HIS:N	1:49:A:HIS:CA	1:49:A:HIS:C	2	1.82
(1,190)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:ARG:N	2	1.8
(1,116)	1:27:A:TRP:N	1:27:A:TRP:CA	1:27:A:TRP:C	1:28:A:GLN:N	4	1.73
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	8	1.71
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	5	1.66
(1,110)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:THR:N	4	1.66
(1,178)	1:101:A:THR:N	1:101:A:THR:CA	1:101:A:THR:C	1:102:A:SER:N	8	1.65
(1,18)	1:22:A:ASP:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	10	1.57
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	10	1.55
(1,94)	1:111:A:ARG:C	1:112:A:GLN:N	1:112:A:GLN:CA	1:112:A:GLN:C	6	1.49
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	8	1.46
(1,18)	1:22:A:ASP:C	1:23:A:GLN:N	1:23:A:GLN:CA	1:23:A:GLN:C	2	1.46
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	3	1.38
(1,45)	1:52:A:LEU:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	6	1.34
(1,78)	1:95:A:ALA:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	2	1.31
(1,95)	1:112:A:GLN:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	2	1.3
(1,81)	1:98:A:LYS:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	6	1.3
(1,175)	1:98:A:LYS:N	1:98:A:LYS:CA	1:98:A:LYS:C	1:99:A:THR:N	2	1.25
(1,81)	1:98:A:LYS:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	3	1.21
(1,178)	1:101:A:THR:N	1:101:A:THR:CA	1:101:A:THR:C	1:102:A:SER:N	7	1.19
(1,15)	1:18:A:PHE:C	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1	1.18
(1,144)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:PRO:N	8	1.12
(1,15)	1:18:A:PHE:C	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	4	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:ASP:N	5	1.08
(1,95)	1:112:A:GLN:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	4	1.05
(1,178)	1:101:A:THR:N	1:101:A:THR:CA	1:101:A:THR:C	1:102:A:SER:N	5	1.04