



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 04:56 PM EST

PDB ID : 6ZV4
BMRB ID : 34541
Title : Human TFIIS N-terminal domain in complex with IWS1
Authors : Veverka, V.
Deposited on : 2020-07-23

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

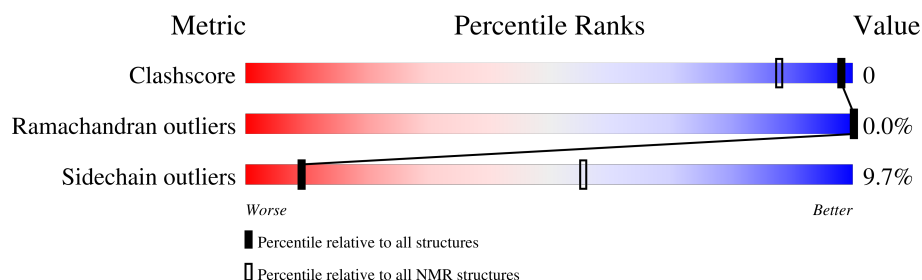
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 94%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	116	

2 Ensemble composition and analysis ⓘ

This entry contains 40 models. Model 37 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:77, A:100-A:104 (81)	0.21	37

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 5, 6, 7, 9, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 30, 31, 32, 34, 35, 36, 37, 38, 39, 40
2	3, 8, 10
3	4, 28, 33
4	14, 29
5	2, 27

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1766 atoms, of which 889 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription elongation factor A protein 1,Protein IWS1 homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1766	534	889	150	188	5	

There are 14 discrepancies between the modelled and reference sequences:

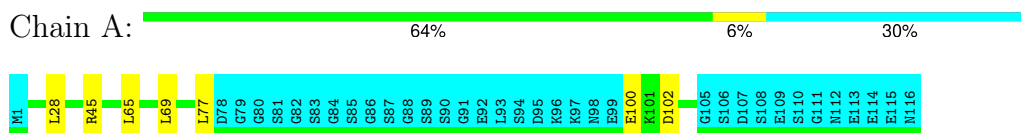
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ASP	-	linker	UNP P23193
A	79	GLY	-	linker	UNP P23193
A	80	GLY	-	linker	UNP P23193
A	81	SER	-	linker	UNP P23193
A	82	GLY	-	linker	UNP P23193
A	83	SER	-	linker	UNP P23193
A	84	GLY	-	linker	UNP P23193
A	85	SER	-	linker	UNP P23193
A	86	GLY	-	linker	UNP P23193
A	87	SER	-	linker	UNP P23193
A	88	GLY	-	linker	UNP P23193
A	89	SER	-	linker	UNP P23193
A	90	SER	-	linker	UNP P23193
A	91	GLY	-	linker	UNP P23193

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: Transcription elongation factor A protein 1,Protein IWS1 homolog

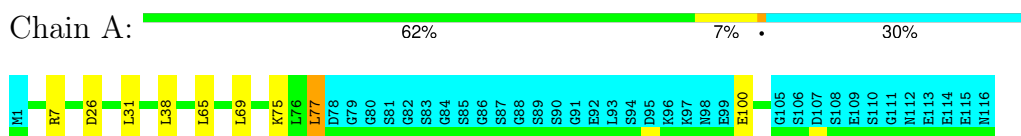


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

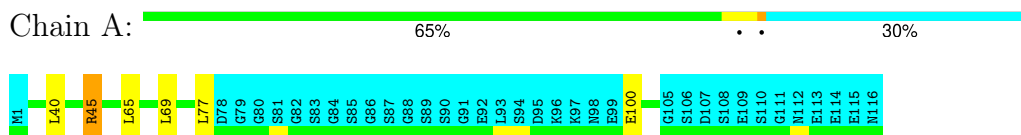
4.2.1 Score per residue for model 1

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



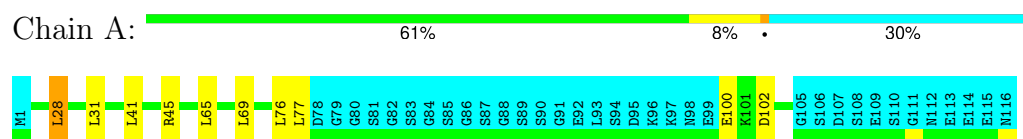
4.2.2 Score per residue for model 2

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



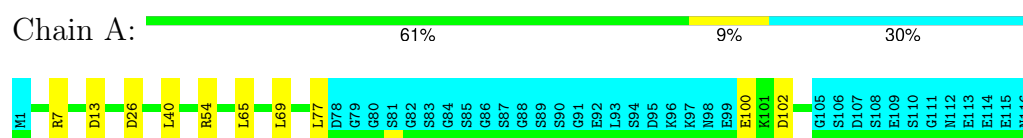
4.2.3 Score per residue for model 3

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



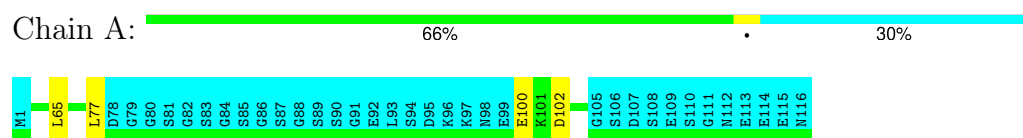
4.2.4 Score per residue for model 4

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



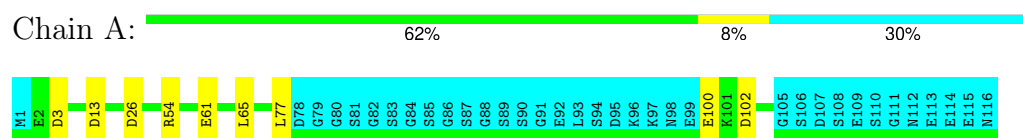
4.2.5 Score per residue for model 5

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



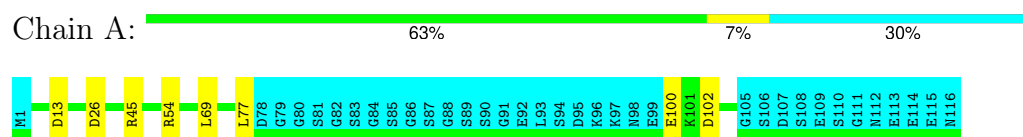
4.2.6 Score per residue for model 6

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



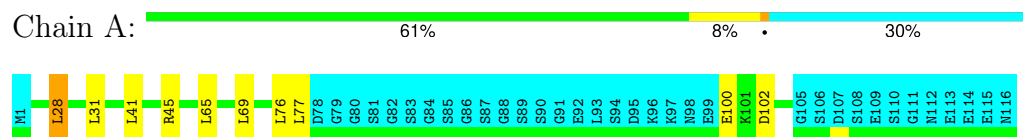
4.2.7 Score per residue for model 7

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



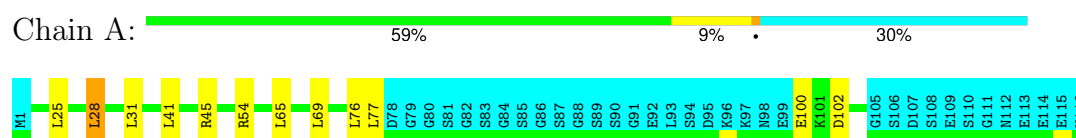
4.2.8 Score per residue for model 8

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



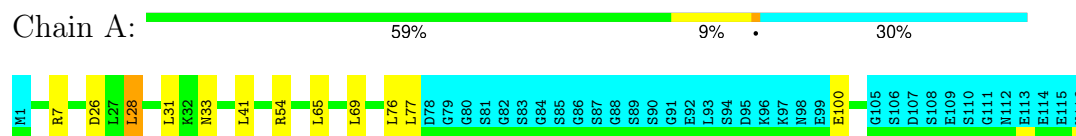
4.2.9 Score per residue for model 9

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



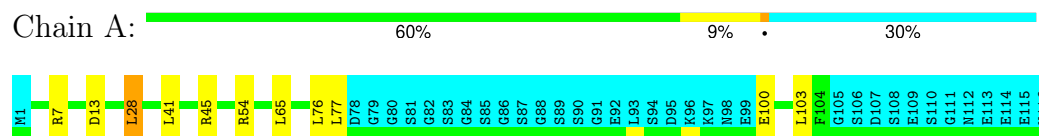
4.2.10 Score per residue for model 10

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



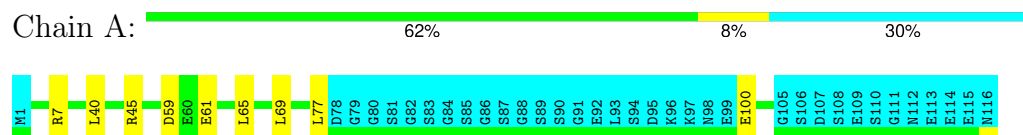
4.2.11 Score per residue for model 11

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



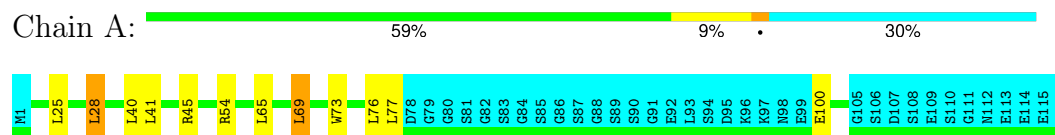
4.2.12 Score per residue for model 12

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



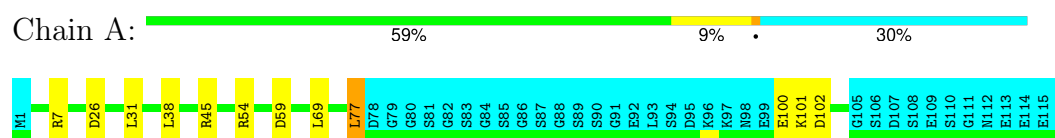
4.2.13 Score per residue for model 13

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



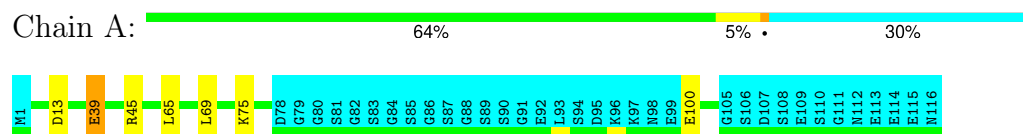
4.2.14 Score per residue for model 14

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



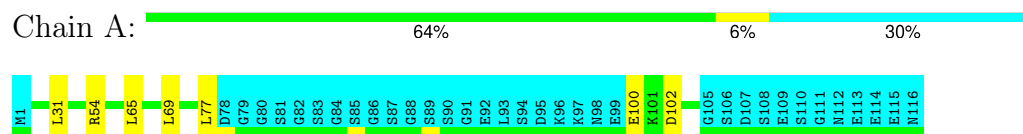
4.2.15 Score per residue for model 15

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



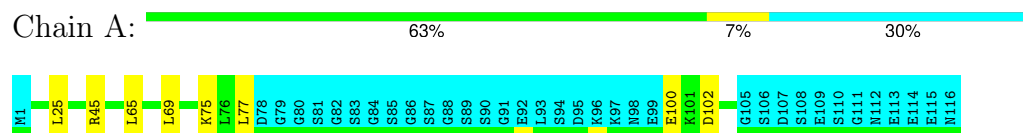
4.2.16 Score per residue for model 16

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



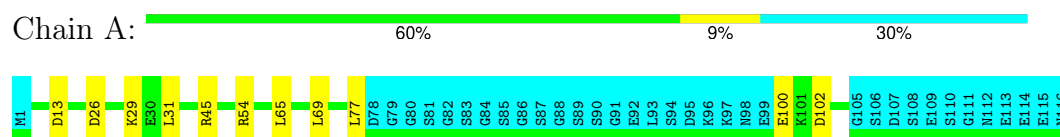
4.2.17 Score per residue for model 17

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



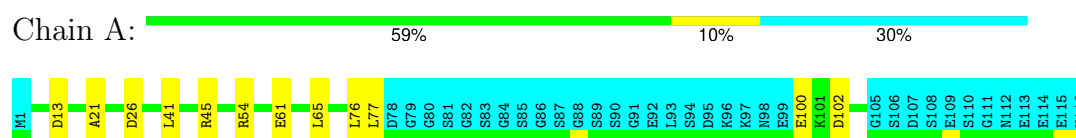
4.2.18 Score per residue for model 18

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



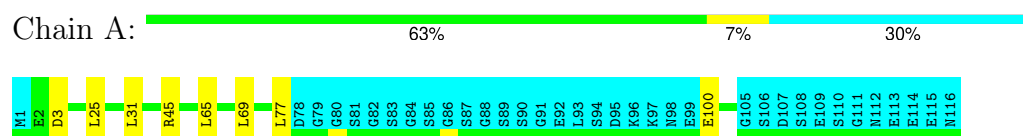
4.2.19 Score per residue for model 19

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



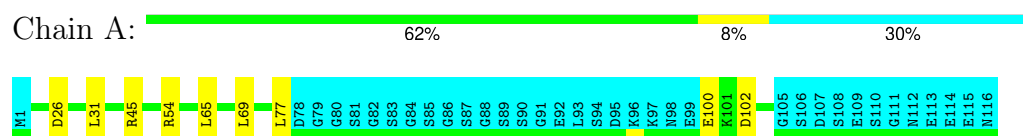
4.2.20 Score per residue for model 20

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



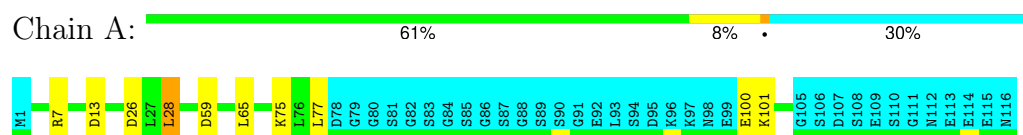
4.2.21 Score per residue for model 21

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



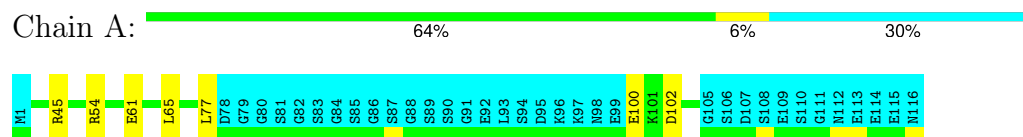
4.2.22 Score per residue for model 22

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



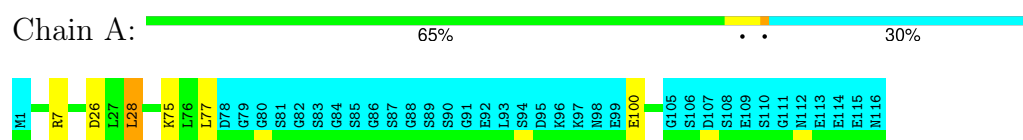
4.2.23 Score per residue for model 23

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



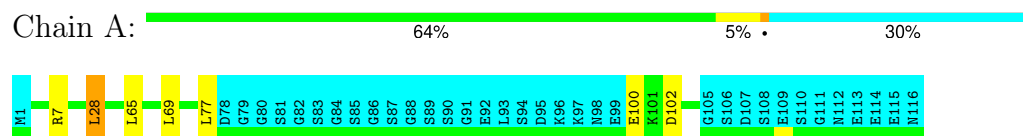
4.2.24 Score per residue for model 24

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



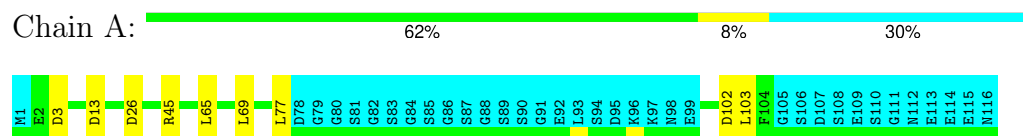
4.2.25 Score per residue for model 25

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



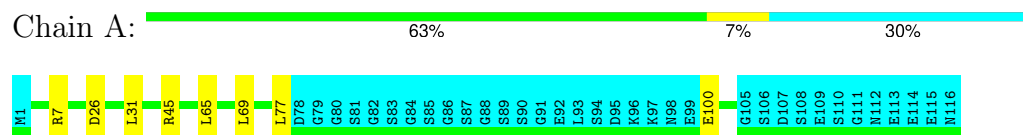
4.2.26 Score per residue for model 26

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



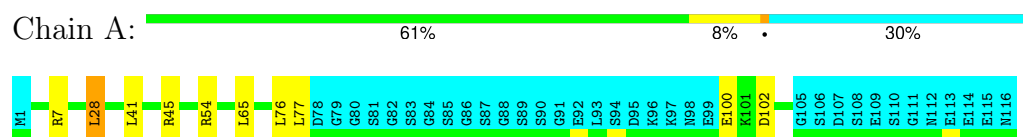
4.2.27 Score per residue for model 27

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



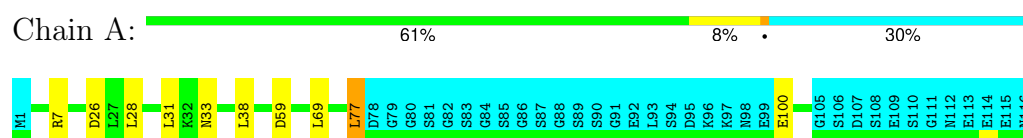
4.2.28 Score per residue for model 28

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



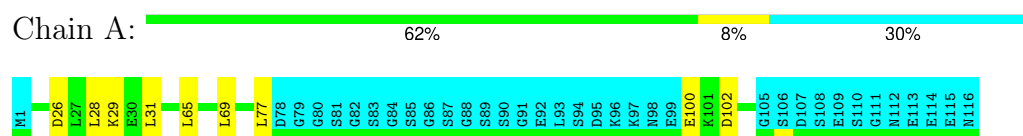
4.2.29 Score per residue for model 29

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



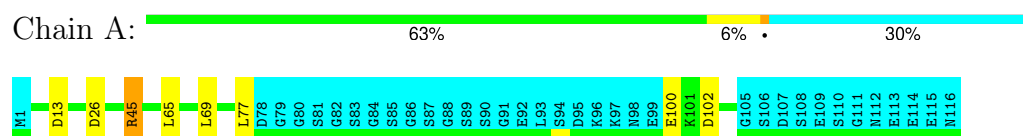
4.2.30 Score per residue for model 30

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



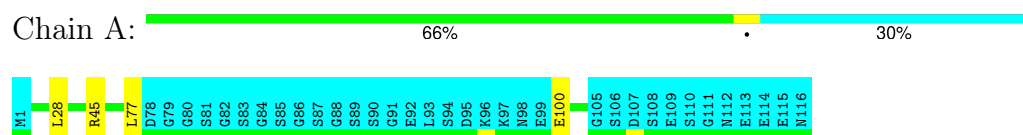
4.2.31 Score per residue for model 31

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



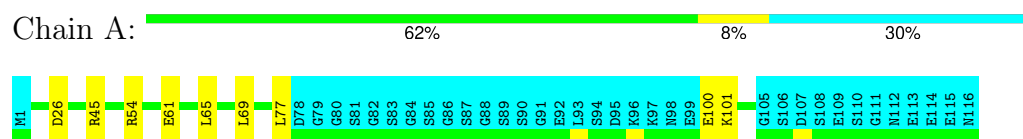
4.2.32 Score per residue for model 32

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



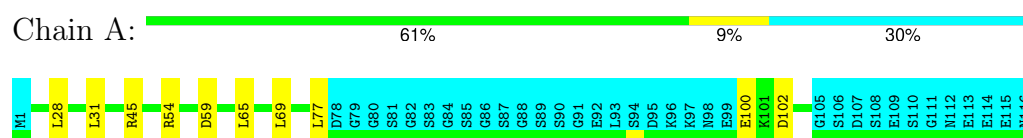
4.2.33 Score per residue for model 33

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



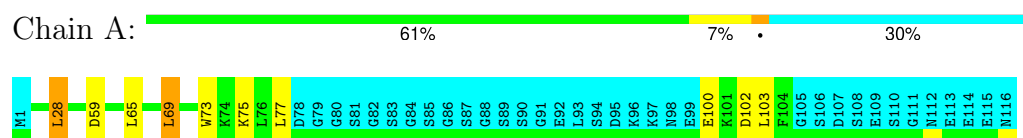
4.2.34 Score per residue for model 34

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



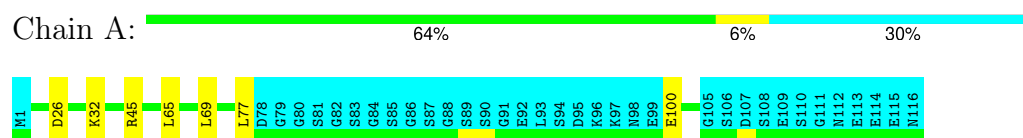
4.2.35 Score per residue for model 35

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



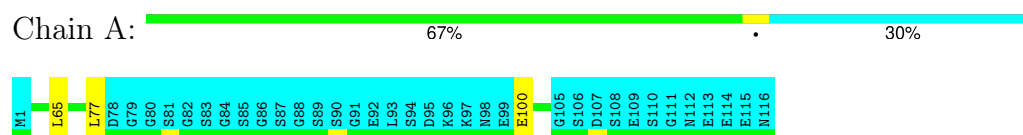
4.2.36 Score per residue for model 36

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



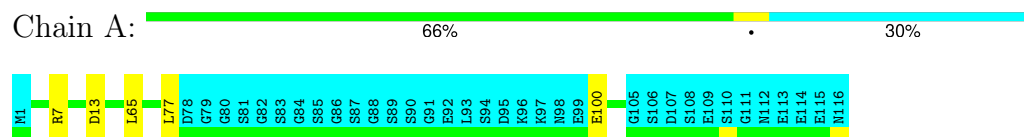
4.2.37 Score per residue for model 37 (medoid)

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



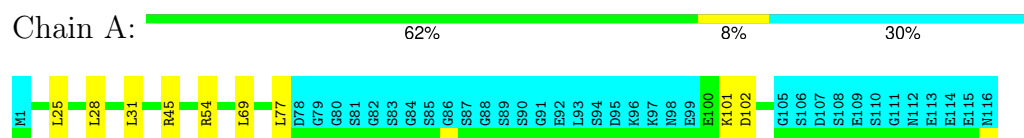
4.2.38 Score per residue for model 38

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



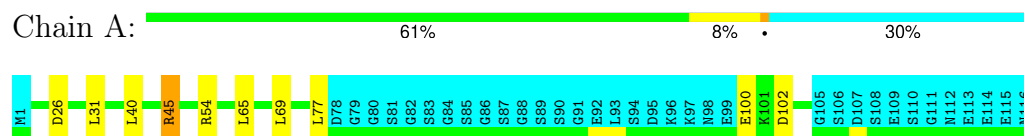
4.2.39 Score per residue for model 39

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



4.2.40 Score per residue for model 40

- Molecule 1: Transcription elongation factor A protein 1,Protein IWS1 homolog



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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
CYANA	structure calculation	
YASARA	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	1304
Number of shifts mapped to atoms	1304
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.59±0.02	0±0/649 (0.0± 0.0%)	0.73±0.03	1±1/866 (0.2± 0.1%)
All	All	0.59	0/25960 (0.0%)	0.73	57/34640 (0.2%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	ARG	NE-CZ-NH1	7.17	123.89	120.30	25	13
1	A	45	ARG	NE-CZ-NH1	7.04	123.82	120.30	40	16
1	A	54	ARG	NE-CZ-NH1	6.39	123.50	120.30	18	17
1	A	28	LEU	CB-CG-CD1	5.46	120.29	111.00	24	11

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	644	698	698	0±1
All	All	25760	27920	27920	14

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD11	1:A:76:LEU:HD12	0.46	1.87	10	8
1:A:38:LEU:HD13	1:A:77:LEU:HB3	0.44	1.87	14	3
1:A:69:LEU:HG	1:A:73:TRP:CZ2	0.41	2.50	13	2
1:A:39:GLU:CD	1:A:39:GLU:H	0.40	2.20	15	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	81/116 (70%)	80±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	3240/4640 (70%)	3196 (99%)	43 (1%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	21	ALA	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	73/99 (74%)	66±2 (90±2%)	7±2 (10±2%)	9	55
All	All	2920/3960 (74%)	2638 (90%)	282 (10%)	9	55

All 23 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	77	LEU	39
1	A	100	GLU	38

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Mol	Chain	Res	Type	Models (Total)
1	A	65	LEU	34
1	A	69	LEU	29
1	A	102	ASP	23
1	A	26	ASP	19
1	A	31	LEU	16
1	A	28	LEU	16
1	A	45	ARG	13
1	A	13	ASP	11
1	A	75	LYS	6
1	A	59	ASP	6
1	A	40	LEU	5
1	A	61	GLU	5
1	A	25	LEU	5
1	A	101	LYS	4
1	A	3	ASP	3
1	A	103	LEU	3
1	A	33	ASN	2
1	A	29	LYS	2
1	A	54	ARG	1
1	A	39	GLU	1
1	A	32	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [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 94% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	1304
Number of shifts mapped to atoms	1304
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	-0.61 ± 0.07	Should be checked
$^{13}\text{C}_\beta$	96	0.09 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	102	-0.54 ± 0.08	Should be applied
^{15}N	100	0.19 ± 0.20	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 94%, i.e. 1091 atoms were assigned a chemical shift out of a possible 1162. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	405/405 (100%)	163/163 (100%)	162/162 (100%)	80/80 (100%)
Sidechain	658/725 (91%)	453/470 (96%)	199/227 (88%)	6/28 (21%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	28/32 (88%)	16/16 (100%)	11/15 (73%)	1/1 (100%)
Overall	1091/1162 (94%)	632/649 (97%)	372/404 (92%)	87/109 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1301 atoms were assigned a chemical shift out of a possible 1500. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	514/589 (87%)	209/242 (86%)	205/232 (88%)	100/115 (87%)
Sidechain	759/879 (86%)	521/564 (92%)	231/282 (82%)	7/33 (21%)
Aromatic	28/32 (88%)	16/16 (100%)	11/15 (73%)	1/1 (100%)
Overall	1301/1500 (87%)	746/822 (91%)	447/529 (84%)	108/149 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

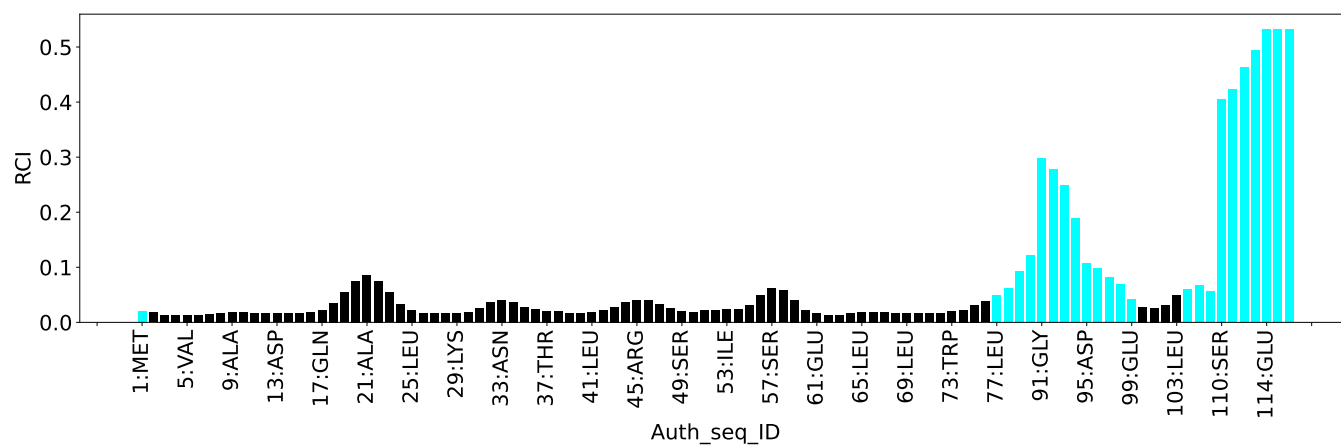
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	37	THR	HG1	5.66	0.08 – 2.19	21.4
1	A	44	THR	HG1	4.58	0.08 – 2.19	16.3
1	A	69	LEU	HB2	-0.15	-0.07 – 3.30	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2893
Intra-residue ($ i-j =0$)	596
Sequential ($ i-j =1$)	603
Medium range ($ i-j >1$ and $ i-j <5$)	741
Long range ($ i-j \geq 5$)	953
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	162
Number of unmapped restraints	0
Number of restraints per residue	26.3
Number of long range restraints per residue ¹	8.2

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)	22.3	0.2
0.2-0.5 (Medium)	9.5	0.5
>0.5 (Large)	3.0	1.58

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)	3.5	5.06
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

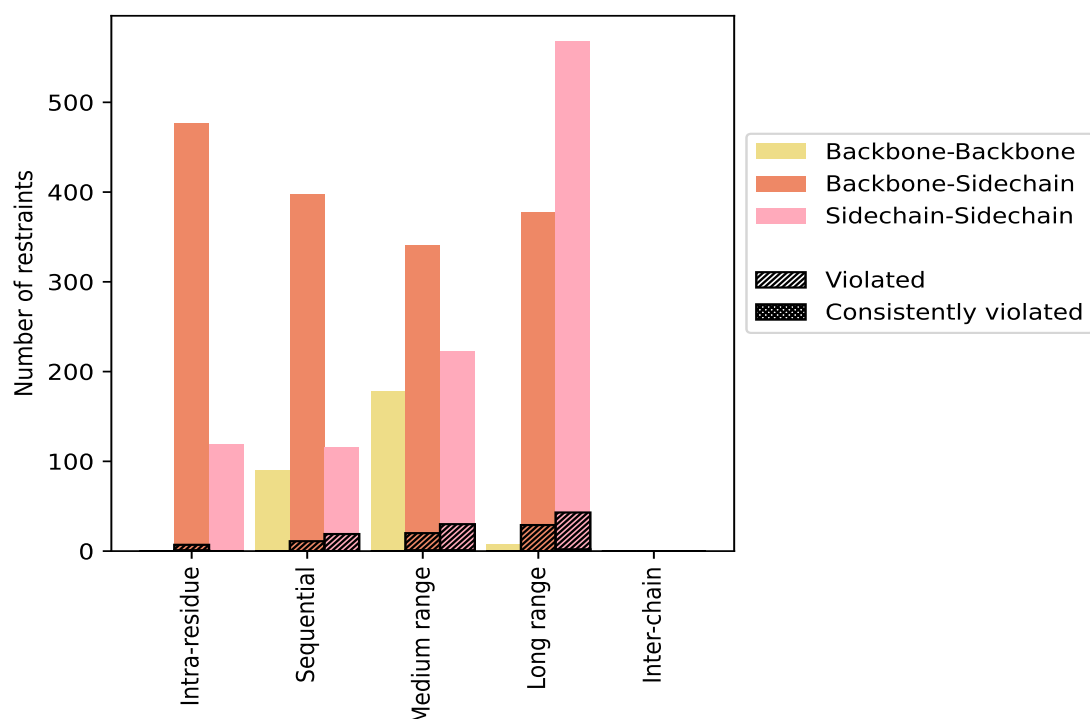
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	596	20.6	7	1.2	0.2	1	0.2	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	477	16.5	7	1.5	0.2	1	0.2	0.0
Sidechain-Sidechain	119	4.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	603	20.8	30	5.0	1.0	0	0.0	0.0
Backbone-Backbone	90	3.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	397	13.7	11	2.8	0.4	0	0.0	0.0
Sidechain-Sidechain	116	4.0	19	16.4	0.7	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	741	25.6	50	6.7	1.7	2	0.3	0.1
Backbone-Backbone	178	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	341	11.8	20	5.9	0.7	1	0.3	0.0
Sidechain-Sidechain	222	7.7	30	13.5	1.0	1	0.5	0.0
Long range ($i-j \geq 5$)	953	32.9	72	7.6	2.5	2	0.2	0.1
Backbone-Backbone	8	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	377	13.0	29	7.7	1.0	0	0.0	0.0
Sidechain-Sidechain	568	19.6	43	7.6	1.5	2	0.4	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2893	100.0	159	5.5	5.5	5	0.2	0.2
Backbone-Backbone	276	9.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1592	55.0	67	4.2	2.3	2	0.1	0.1
Sidechain-Sidechain	1025	35.4	92	9.0	3.2	3	0.3	0.1

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	2	2	6	10	0	20	0.33	1.49	0.38	0.17
2	1	4	10	15	0	30	0.28	1.5	0.34	0.14
3	1	1	3	5	0	10	0.55	1.49	0.51	0.32
4	2	3	17	22	0	44	0.24	1.53	0.27	0.15
5	2	5	8	10	0	25	0.29	1.45	0.34	0.18
6	1	7	16	21	0	45	0.24	1.5	0.28	0.15
7	2	4	20	24	0	50	0.24	1.49	0.27	0.15
8	1	2	5	7	0	15	0.37	1.49	0.45	0.15
9	1	1	5	4	0	11	0.45	1.48	0.48	0.2
10	1	1	6	5	0	13	0.37	1.49	0.46	0.13

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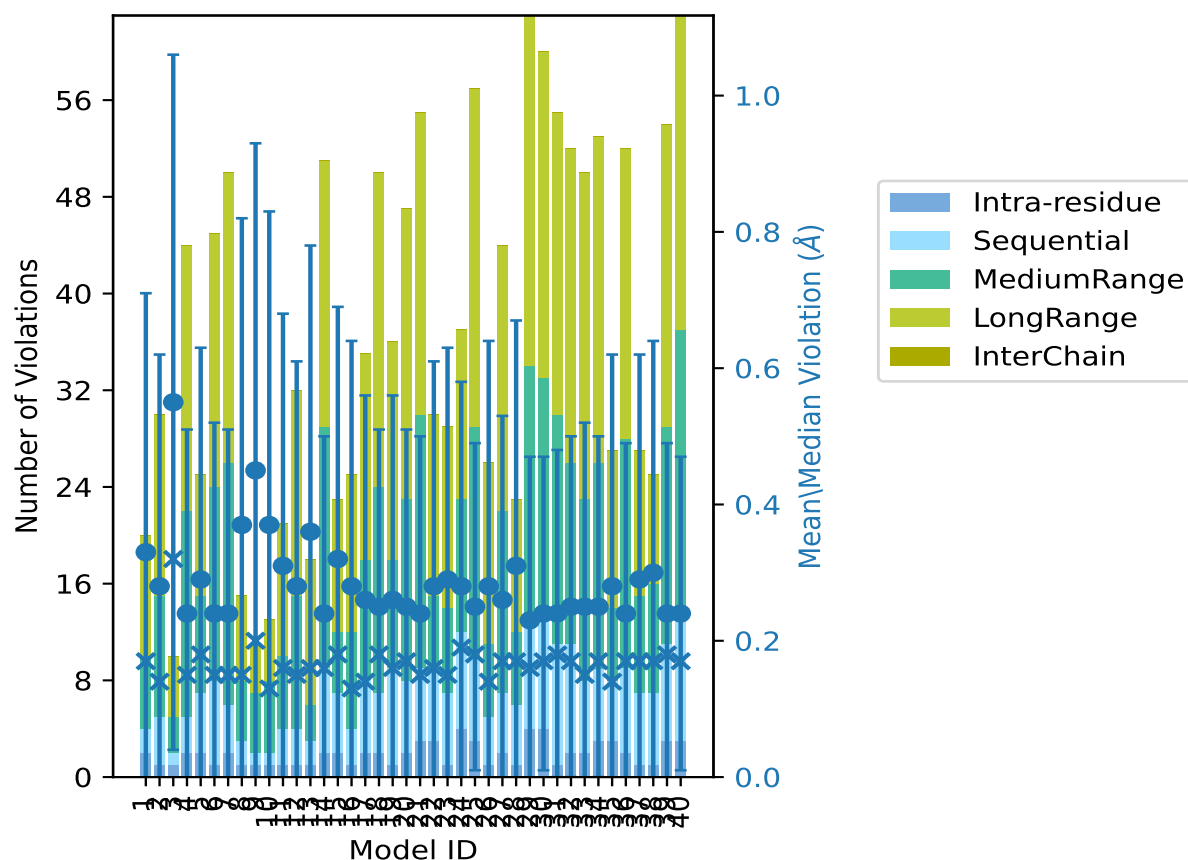
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	3	6	11	0	21	0.31	1.44	0.37	0.16
12	1	3	11	17	0	32	0.28	1.5	0.33	0.15
13	1	2	3	12	0	18	0.36	1.44	0.42	0.16
14	2	7	20	22	0	51	0.24	1.56	0.26	0.16
15	2	5	5	11	0	23	0.32	1.5	0.37	0.18
16	1	3	8	13	0	25	0.28	1.48	0.36	0.13
17	2	6	10	17	0	35	0.26	1.47	0.3	0.14
18	2	5	17	26	0	50	0.25	1.52	0.26	0.18
19	1	8	9	18	0	36	0.26	1.49	0.3	0.16
20	2	6	15	24	0	47	0.25	1.52	0.26	0.17
21	3	6	21	25	0	55	0.24	1.51	0.26	0.15
22	3	6	6	15	0	30	0.28	1.49	0.33	0.16
23	1	6	7	15	0	29	0.29	1.49	0.34	0.15
24	4	8	11	14	0	37	0.28	1.48	0.3	0.19
25	3	7	19	28	0	57	0.25	1.5	0.24	0.18
26	1	4	6	15	0	26	0.28	1.5	0.36	0.14
27	2	5	15	22	0	44	0.26	1.55	0.27	0.17
28	1	5	6	11	0	23	0.31	1.48	0.36	0.17
29	4	9	21	29	0	63	0.23	1.58	0.24	0.16
30	4	9	20	27	0	60	0.24	1.5	0.23	0.17
31	1	10	19	25	0	55	0.24	1.47	0.24	0.18
32	2	9	15	26	0	52	0.25	1.52	0.25	0.17
33	2	6	15	27	0	50	0.25	1.5	0.27	0.15
34	3	6	17	27	0	53	0.25	1.51	0.25	0.17
35	3	5	6	13	0	27	0.28	1.47	0.34	0.14
36	2	7	19	24	0	52	0.24	1.54	0.25	0.17
37	1	6	8	12	0	27	0.29	1.47	0.33	0.17
38	1	6	9	9	0	25	0.3	1.47	0.34	0.17
39	3	8	18	25	0	54	0.24	1.48	0.25	0.18
40	3	11	23	26	0	63	0.24	1.56	0.23	0.17

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2734(IR:589, SQ:573, MR:691, LR:881, 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	%
1	7	19	17	0	44	1	2.5
1	5	4	5	0	15	2	5.0
1	3	2	7	0	13	3	7.5
0	1	2	5	0	8	4	10.0
0	1	1	3	0	5	5	12.5
0	4	2	6	0	12	6	15.0

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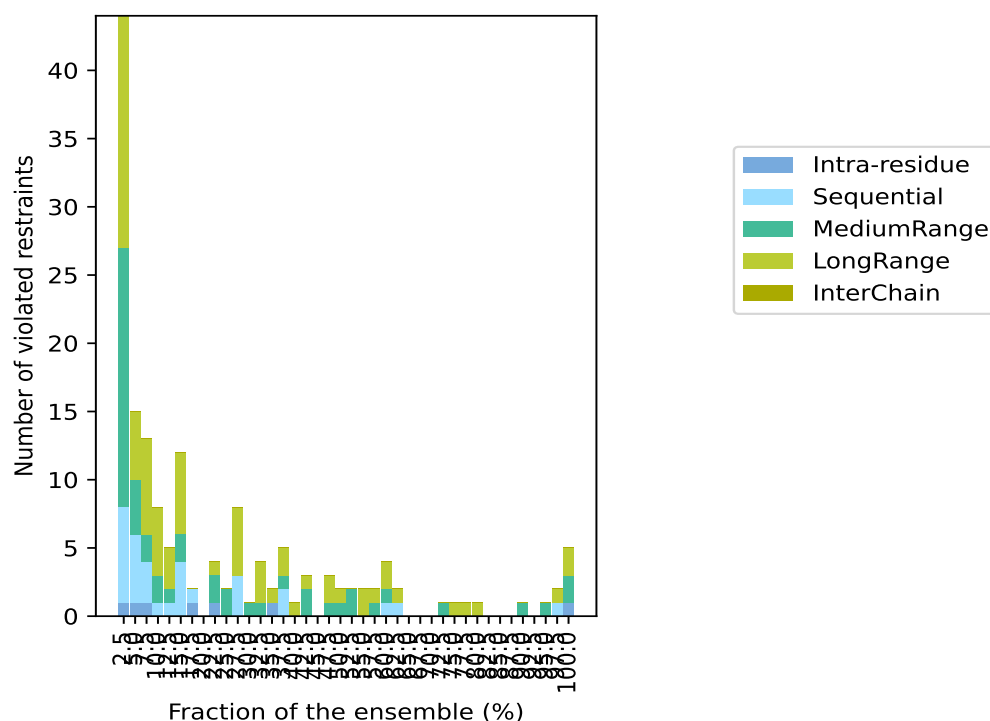
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	0	0	0	2	7	17.5
0	0	0	0	0	0	8	20.0
1	0	2	1	0	4	9	22.5
0	0	2	0	0	2	10	25.0
0	3	0	5	0	8	11	27.5
0	0	1	0	0	1	12	30.0
0	0	1	3	0	4	13	32.5
1	0	0	1	0	2	14	35.0
0	2	1	2	0	5	15	37.5
0	0	0	1	0	1	16	40.0
0	0	2	1	0	3	17	42.5
0	0	0	0	0	0	18	45.0
0	0	1	2	0	3	19	47.5
0	0	1	1	0	2	20	50.0
0	0	2	0	0	2	21	52.5
0	0	0	2	0	2	22	55.0
0	0	1	1	0	2	23	57.5
0	1	1	2	0	4	24	60.0
0	1	0	1	0	2	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	1	0	0	1	29	72.5
0	0	0	1	0	1	30	75.0
0	0	0	1	0	1	31	77.5
0	0	0	1	0	1	32	80.0
0	0	0	0	0	0	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	1	0	0	1	36	90.0
0	0	0	0	0	0	37	92.5
0	0	1	0	0	1	38	95.0
0	1	0	1	0	2	39	97.5
1	0	2	2	0	5	40	100.0

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

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

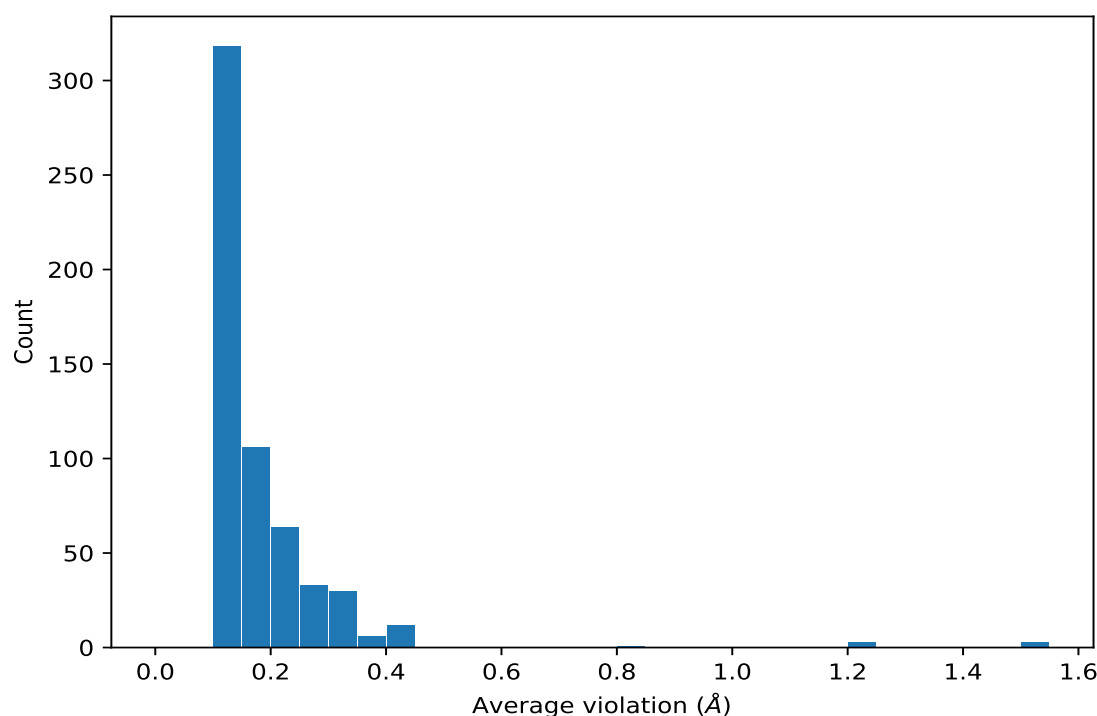
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	40	1.5	0.03	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	40	1.5	0.03	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	40	1.5	0.03	1.49
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	40	1.22	0.09	1.21
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	40	1.22	0.09	1.21
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	40	1.22	0.09	1.21
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	40	0.85	0.06	0.86
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	40	0.34	0.09	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	40	0.34	0.09	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	40	0.34	0.09	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	40	0.34	0.09	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	40	0.34	0.09	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	40	0.34	0.09	0.32
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	40	0.26	0.09	0.24
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	40	0.26	0.09	0.24
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	40	0.26	0.09	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	39	0.31	0.13	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	39	0.31	0.13	0.29
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	39	0.23	0.07	0.22
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	39	0.23	0.07	0.22
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	39	0.23	0.07	0.22
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	38	0.32	0.1	0.31
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	38	0.32	0.1	0.31
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	38	0.32	0.1	0.31
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	38	0.32	0.1	0.31
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	38	0.32	0.1	0.31
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	38	0.32	0.1	0.31
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	36	0.15	0.04	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	36	0.15	0.04	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	36	0.15	0.04	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	36	0.15	0.04	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	36	0.15	0.04	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	36	0.15	0.04	0.15
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	32	0.15	0.04	0.15
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	32	0.15	0.04	0.15
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	32	0.15	0.04	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	31	0.17	0.05	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	31	0.17	0.05	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	31	0.17	0.05	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	31	0.17	0.05	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	31	0.17	0.05	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	31	0.17	0.05	0.16
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	30	0.16	0.05	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	30	0.16	0.05	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	30	0.16	0.05	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	30	0.16	0.05	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	30	0.16	0.05	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	30	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	29	0.14	0.03	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	29	0.14	0.03	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	29	0.14	0.03	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	29	0.14	0.03	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	29	0.14	0.03	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	29	0.14	0.03	0.14
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	25	0.2	0.07	0.19
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	25	0.14	0.03	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	25	0.14	0.03	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	25	0.14	0.03	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	24	0.2	0.05	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	24	0.2	0.05	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	24	0.2	0.05	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	24	0.2	0.05	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	24	0.2	0.05	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	24	0.2	0.05	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	24	0.17	0.04	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	24	0.17	0.04	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	24	0.17	0.04	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	24	0.17	0.04	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	24	0.17	0.04	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	24	0.17	0.04	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	24	0.17	0.04	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	24	0.17	0.04	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	24	0.17	0.04	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	24	0.16	0.04	0.16
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	24	0.16	0.04	0.16
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	24	0.16	0.04	0.16
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	23	0.25	0.08	0.26
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	23	0.25	0.08	0.26
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	23	0.25	0.08	0.26
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	23	0.22	0.08	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	23	0.22	0.08	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	23	0.22	0.08	0.23
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	22	0.15	0.03	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	22	0.15	0.03	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	22	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	22	0.15	0.03	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	22	0.15	0.03	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	22	0.15	0.03	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	22	0.14	0.02	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	22	0.14	0.02	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	22	0.14	0.02	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	21	0.15	0.03	0.15
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	21	0.15	0.03	0.15
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	21	0.15	0.03	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	21	0.15	0.03	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	21	0.15	0.03	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	21	0.15	0.03	0.14
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	20	0.17	0.05	0.18
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	20	0.17	0.05	0.18
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	20	0.17	0.05	0.18
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	20	0.15	0.03	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	20	0.15	0.03	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	20	0.15	0.03	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	19	0.15	0.03	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	19	0.15	0.03	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	19	0.15	0.03	0.14
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	19	0.13	0.03	0.13
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	19	0.13	0.03	0.13
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	19	0.13	0.03	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	19	0.13	0.02	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	19	0.13	0.02	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	19	0.13	0.02	0.14
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	17	0.21	0.04	0.23
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	17	0.21	0.04	0.23
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	17	0.21	0.04	0.23
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	17	0.18	0.08	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	17	0.18	0.08	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	17	0.18	0.08	0.14
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	17	0.15	0.04	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	17	0.15	0.04	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	17	0.15	0.04	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	17	0.15	0.04	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	17	0.15	0.04	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	17	0.15	0.04	0.16
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	16	0.22	0.09	0.19
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	16	0.22	0.09	0.19
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	16	0.22	0.09	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	16	0.22	0.09	0.19
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	16	0.22	0.09	0.19
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	16	0.22	0.09	0.19
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	15	0.21	0.11	0.14
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	15	0.21	0.11	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	15	0.16	0.06	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	15	0.16	0.06	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	15	0.16	0.06	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	15	0.16	0.06	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	15	0.16	0.06	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	15	0.16	0.06	0.14
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	15	0.14	0.03	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	15	0.14	0.03	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	15	0.14	0.03	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	15	0.14	0.03	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	15	0.14	0.03	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	15	0.14	0.03	0.13
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	15	0.14	0.06	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	15	0.13	0.02	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	15	0.13	0.02	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	15	0.13	0.02	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	15	0.13	0.02	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	15	0.13	0.02	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	15	0.13	0.02	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	14	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	14	0.19	0.06	0.18
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	14	0.19	0.06	0.18
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	14	0.13	0.02	0.12
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	13	0.38	0.04	0.39
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	13	0.21	0.04	0.21
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	13	0.21	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	13	0.21	0.04	0.21
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	13	0.16	0.05	0.14
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	13	0.16	0.05	0.14
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	13	0.16	0.05	0.14
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	13	0.16	0.05	0.14
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	13	0.15	0.04	0.13
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	13	0.15	0.04	0.13
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	13	0.15	0.04	0.13
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	12	0.17	0.06	0.16
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	12	0.17	0.06	0.16
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	12	0.17	0.06	0.16
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	11	0.34	0.03	0.34
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	11	0.29	0.06	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	11	0.29	0.06	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	11	0.29	0.06	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	11	0.29	0.06	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	11	0.29	0.06	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	11	0.29	0.06	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	11	0.28	0.04	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	11	0.28	0.04	0.29
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	11	0.19	0.05	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	11	0.19	0.05	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	11	0.19	0.05	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	11	0.19	0.05	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	11	0.19	0.05	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	11	0.19	0.05	0.22
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	11	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	11	0.18	0.04	0.18
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	11	0.18	0.04	0.18
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	11	0.13	0.03	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	11	0.13	0.03	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	11	0.13	0.03	0.12
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	11	0.13	0.02	0.13
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	11	0.13	0.02	0.13
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	11	0.13	0.02	0.13
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	11	0.12	0.01	0.11
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	10	0.2	0.04	0.22
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	10	0.2	0.04	0.22
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	10	0.2	0.04	0.22
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	10	0.12	0.02	0.11
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	10	0.12	0.02	0.11
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	10	0.12	0.02	0.11
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	9	0.17	0.05	0.2
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	9	0.15	0.07	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	9	0.14	0.02	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	9	0.14	0.02	0.14
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	9	0.14	0.03	0.14
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	7	0.15	0.03	0.14
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	7	0.15	0.03	0.14
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	7	0.12	0.03	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	7	0.12	0.03	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	7	0.12	0.03	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	7	0.12	0.03	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	7	0.12	0.03	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	7	0.12	0.03	0.11
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	6	0.44	0.06	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	6	0.44	0.06	0.48
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	6	0.25	0.12	0.23
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	6	0.25	0.12	0.23
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	6	0.25	0.12	0.23
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	6	0.16	0.04	0.15
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	6	0.16	0.04	0.15
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	6	0.15	0.05	0.12
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	6	0.15	0.05	0.12
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	6	0.15	0.05	0.12
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	6	0.15	0.05	0.12
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	6	0.15	0.05	0.12
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	6	0.15	0.05	0.12
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	6	0.14	0.04	0.12
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	6	0.14	0.04	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	6	0.14	0.04	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	6	0.14	0.04	0.14
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	6	0.14	0.04	0.14
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	6	0.14	0.04	0.14
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	6	0.14	0.04	0.14
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	6	0.14	0.04	0.14
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	6	0.14	0.02	0.14
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	6	0.14	0.02	0.14
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	6	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	6	0.13	0.02	0.13
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	6	0.13	0.03	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	6	0.13	0.03	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	6	0.13	0.03	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	6	0.13	0.03	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	6	0.13	0.03	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	6	0.13	0.03	0.12
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	6	0.11	0.01	0.11
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	6	0.11	0.01	0.11
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	6	0.11	0.01	0.11
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	6	0.11	0.01	0.11
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	5	0.2	0.15	0.13
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	5	0.2	0.15	0.13
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	5	0.2	0.15	0.13
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	5	0.2	0.15	0.13
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	5	0.14	0.03	0.14
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	5	0.14	0.03	0.14
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	5	0.14	0.03	0.14
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	5	0.12	0.01	0.12
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	5	0.12	0.01	0.12
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	5	0.12	0.01	0.12
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	5	0.12	0.02	0.11
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	5	0.12	0.02	0.11
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	5	0.12	0.02	0.11
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	5	0.11	0.01	0.11
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	5	0.11	0.01	0.11
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	5	0.11	0.01	0.11
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG21	4	0.15	0.03	0.16
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG22	4	0.15	0.03	0.16
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG23	4	0.15	0.03	0.16
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG21	4	0.15	0.03	0.16
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG22	4	0.15	0.03	0.16
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG23	4	0.15	0.03	0.16
(1,439)	1:25:A:LEU:HD11	1:62:A:VAL:H	4	0.15	0.03	0.14
(1,439)	1:25:A:LEU:HD12	1:62:A:VAL:H	4	0.15	0.03	0.14
(1,439)	1:25:A:LEU:HD13	1:62:A:VAL:H	4	0.15	0.03	0.14
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD11	4	0.12	0.03	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD12	4	0.12	0.03	0.11
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD13	4	0.12	0.03	0.11
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD21	4	0.12	0.03	0.11
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD22	4	0.12	0.03	0.11
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD23	4	0.12	0.03	0.11
(1,2844)	1:77:A:LEU:HD11	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,2844)	1:77:A:LEU:HD12	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,2844)	1:77:A:LEU:HD13	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,2844)	1:77:A:LEU:HD21	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,2844)	1:77:A:LEU:HD22	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,2844)	1:77:A:LEU:HD23	1:103:A:LEU:H	4	0.12	0.01	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD11	4	0.12	0.01	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD12	4	0.12	0.01	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD13	4	0.12	0.01	0.12
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD11	4	0.11	0.02	0.11
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD12	4	0.11	0.02	0.11
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD13	4	0.11	0.02	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB1	4	0.11	0.0	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB2	4	0.11	0.0	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB3	4	0.11	0.0	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB1	4	0.11	0.0	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB2	4	0.11	0.0	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB3	4	0.11	0.0	0.11
(1,1166)	1:70:A:ILE:HD11	1:73:A:TRP:HH2	4	0.11	0.01	0.1
(1,1166)	1:70:A:ILE:HD12	1:73:A:TRP:HH2	4	0.11	0.01	0.1
(1,1166)	1:70:A:ILE:HD13	1:73:A:TRP:HH2	4	0.11	0.01	0.1
(1,2364)	1:25:A:LEU:HD11	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,2364)	1:25:A:LEU:HD12	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,2364)	1:25:A:LEU:HD13	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,2364)	1:25:A:LEU:HD21	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,2364)	1:25:A:LEU:HD22	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,2364)	1:25:A:LEU:HD23	1:62:A:VAL:HA	3	0.29	0.06	0.3
(1,1462)	1:77:A:LEU:HD21	1:78:A:ASP:HA	3	0.24	0.08	0.19
(1,1462)	1:77:A:LEU:HD22	1:78:A:ASP:HA	3	0.24	0.08	0.19
(1,1462)	1:77:A:LEU:HD23	1:78:A:ASP:HA	3	0.24	0.08	0.19
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE1	3	0.21	0.08	0.25
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE2	3	0.21	0.08	0.25
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE3	3	0.21	0.08	0.25
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE1	3	0.21	0.08	0.25
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE2	3	0.21	0.08	0.25
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE3	3	0.21	0.08	0.25
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD11	3	0.17	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD12	3	0.17	0.04	0.17
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD13	3	0.17	0.04	0.17
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD11	3	0.16	0.01	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD12	3	0.16	0.01	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD13	3	0.16	0.01	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD21	3	0.16	0.01	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD22	3	0.16	0.01	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD23	3	0.16	0.01	0.15
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD2	3	0.14	0.04	0.14
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD3	3	0.14	0.04	0.14
(1,324)	1:24:A:ALA:HB1	1:62:A:VAL:HB	3	0.14	0.02	0.13
(1,324)	1:24:A:ALA:HB2	1:62:A:VAL:HB	3	0.14	0.02	0.13
(1,324)	1:24:A:ALA:HB3	1:62:A:VAL:HB	3	0.14	0.02	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD11	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD12	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD13	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD11	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD12	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD13	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD11	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD12	3	0.13	0.0	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD13	3	0.13	0.0	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD11	3	0.13	0.02	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD12	3	0.13	0.02	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD13	3	0.13	0.02	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD11	3	0.13	0.02	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD12	3	0.13	0.02	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD13	3	0.13	0.02	0.13
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD11	3	0.12	0.02	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD12	3	0.12	0.02	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD13	3	0.12	0.02	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD21	3	0.12	0.02	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD22	3	0.12	0.02	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD23	3	0.12	0.02	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB1	3	0.12	0.01	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB2	3	0.12	0.01	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB3	3	0.12	0.01	0.12
(1,1119)	1:69:A:LEU:HD11	1:73:A:TRP:HE3	3	0.12	0.01	0.12
(1,1119)	1:69:A:LEU:HD12	1:73:A:TRP:HE3	3	0.12	0.01	0.12
(1,1119)	1:69:A:LEU:HD13	1:73:A:TRP:HE3	3	0.12	0.01	0.12
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB1	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB2	3	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB3	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB1	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB2	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB3	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB1	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB2	3	0.11	0.01	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB3	3	0.11	0.01	0.1
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD11	2	0.21	0.02	0.21
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD12	2	0.21	0.02	0.21
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD13	2	0.21	0.02	0.21
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD21	2	0.21	0.02	0.21
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD22	2	0.21	0.02	0.21
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD23	2	0.21	0.02	0.21
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD11	2	0.19	0.07	0.19
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD12	2	0.19	0.07	0.19
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD13	2	0.19	0.07	0.19
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD21	2	0.19	0.07	0.19
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD22	2	0.19	0.07	0.19
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD23	2	0.19	0.07	0.19
(1,2725)	1:59:A:ASP:HB2	1:62:A:VAL:HB	2	0.14	0.01	0.14
(1,2725)	1:59:A:ASP:HB3	1:62:A:VAL:HB	2	0.14	0.01	0.14
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB2	2	0.14	0.02	0.14
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB3	2	0.14	0.02	0.14
(1,1617)	1:14:A:LYS:HB2	1:15:A:MET:H	2	0.13	0.0	0.13
(1,1617)	1:14:A:LYS:HB3	1:15:A:MET:H	2	0.13	0.0	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG22	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG22	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG22	2	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG22	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG22	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG11	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG12	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG13	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG21	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG22	2	0.13	0.01	0.13
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG23	2	0.13	0.01	0.13
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG21	2	0.12	0.02	0.12
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG22	2	0.12	0.02	0.12
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG23	2	0.12	0.02	0.12
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG11	2	0.12	0.01	0.12
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG12	2	0.12	0.01	0.12
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG13	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	2	0.12	0.01	0.12
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG11	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG12	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG13	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG21	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG22	2	0.12	0.01	0.12
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG23	2	0.12	0.01	0.12
(1,1453)	1:101:A:LYS:HG2	1:102:A:ASP:HB3	2	0.12	0.02	0.12
(1,1453)	1:101:A:LYS:HG3	1:102:A:ASP:HB3	2	0.12	0.02	0.12

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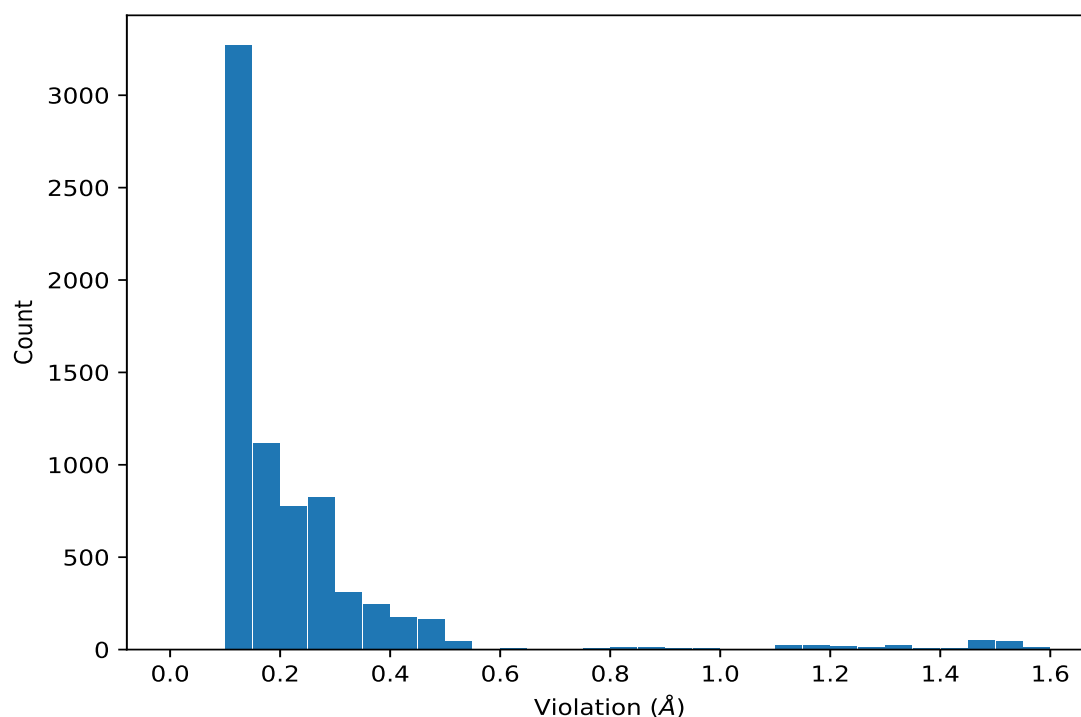
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB2	2	0.12	0.0	0.12
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB3	2	0.12	0.0	0.12
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB2	2	0.12	0.0	0.12
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB3	2	0.12	0.0	0.12
(1,313)	1:24:A:ALA:HB1	1:53:A:ILE:H	2	0.11	0.01	0.11
(1,313)	1:24:A:ALA:HB2	1:53:A:ILE:H	2	0.11	0.01	0.11
(1,313)	1:24:A:ALA:HB3	1:53:A:ILE:H	2	0.11	0.01	0.11
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD11	2	0.11	0.01	0.11
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD12	2	0.11	0.01	0.11
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD13	2	0.11	0.01	0.11
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB2	2	0.11	0.01	0.11
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB3	2	0.11	0.01	0.11
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB2	2	0.11	0.01	0.11
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB3	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	29	1.58
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	29	1.58
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	29	1.58
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	14	1.56
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	14	1.56
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	14	1.56
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	40	1.56
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	40	1.56
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	40	1.56
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	27	1.55
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	27	1.55
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	27	1.55
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	36	1.54
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	36	1.54
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	36	1.54
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	4	1.53
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	4	1.53
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	4	1.53
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	18	1.52
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	18	1.52
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	18	1.52
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	20	1.52
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	20	1.52
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	20	1.52
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	32	1.52
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	32	1.52
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	32	1.52
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	21	1.51
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	21	1.51
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	21	1.51
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	34	1.51
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	34	1.51
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	34	1.51
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	2	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	2	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	2	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	6	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	6	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	6	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	12	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	12	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	12	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	15	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	15	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	15	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	25	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	25	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	25	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	26	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	26	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	26	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	30	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	30	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	30	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	33	1.5
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	33	1.5
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	33	1.5
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	1	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	1	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	1	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	3	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	3	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	3	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	7	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	7	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	7	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	8	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	8	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	8	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	10	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	10	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	10	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	19	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	19	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	19	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	22	1.49
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	22	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	22	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	23	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	23	1.49
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	23	1.49
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	9	1.48
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	9	1.48
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	9	1.48
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	16	1.48
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	16	1.48
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	16	1.48
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	24	1.48
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	24	1.48
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	24	1.48
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	28	1.48
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	28	1.48
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	28	1.48
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	39	1.48
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	39	1.48
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	39	1.48
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	17	1.47
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	17	1.47
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	17	1.47
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	31	1.47
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	31	1.47
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	31	1.47
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	35	1.47
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	35	1.47
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	35	1.47
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	37	1.47
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	37	1.47
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	37	1.47
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	38	1.47
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	38	1.47
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	38	1.47
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	5	1.45
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	5	1.45
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	5	1.45
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	11	1.44
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	11	1.44
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	11	1.44
(1,2093)	1:53:A:ILE:HD11	1:56:A:GLN:HE21	13	1.44
(1,2093)	1:53:A:ILE:HD12	1:56:A:GLN:HE21	13	1.44
(1,2093)	1:53:A:ILE:HD13	1:56:A:GLN:HE21	13	1.44
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	13	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	13	1.39
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	13	1.39
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	3	1.37
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	3	1.37
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	3	1.37
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	15	1.34
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	15	1.34
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	15	1.34
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	8	1.33
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	8	1.33
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	8	1.33
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	16	1.33
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	16	1.33
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	16	1.33
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	23	1.33
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	23	1.33
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	23	1.33
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	24	1.33
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	24	1.33
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	24	1.33
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	12	1.32
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	12	1.32
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	12	1.32
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	21	1.31
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	21	1.31
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	21	1.31
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	26	1.31
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	26	1.31
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	26	1.31
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	22	1.29
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	22	1.29
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	22	1.29
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	7	1.28
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	7	1.28
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	7	1.28
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	9	1.27
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	9	1.27
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	9	1.27
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	37	1.25
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	37	1.25
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	37	1.25
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	1	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	1	1.24
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	1	1.24
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	2	1.24
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	2	1.24
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	2	1.24
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	5	1.23
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	5	1.23
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	5	1.23
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	6	1.23
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	6	1.23
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	6	1.23
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	4	1.22
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	4	1.22
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	4	1.22
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	10	1.22
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	10	1.22
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	10	1.22
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	19	1.21
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	19	1.21
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	19	1.21
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	31	1.2
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	31	1.2
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	31	1.2
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	35	1.2
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	35	1.2
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	35	1.2
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	11	1.18
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	11	1.18
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	11	1.18
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	28	1.17
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	28	1.17
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	28	1.17
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	33	1.17
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	33	1.17
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	33	1.17
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	38	1.17
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	38	1.17
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	38	1.17
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	14	1.16
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	14	1.16
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	14	1.16
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	17	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	17	1.16
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	17	1.16
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	18	1.15
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	18	1.15
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	18	1.15
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	39	1.15
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	39	1.15
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	39	1.15
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	25	1.14
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	25	1.14
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	25	1.14
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	29	1.14
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	29	1.14
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	29	1.14
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	36	1.14
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	36	1.14
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	36	1.14
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	20	1.12
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	20	1.12
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	20	1.12
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	27	1.12
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	27	1.12
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	27	1.12
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	30	1.12
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	30	1.12
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	30	1.12
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	32	1.1
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	32	1.1
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	32	1.1
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	40	1.05
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	40	1.05
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	40	1.05
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	34	0.98
(1,296)	1:21:A:ALA:HB1	1:56:A:GLN:HE21	34	0.98
(1,296)	1:21:A:ALA:HB2	1:56:A:GLN:HE21	34	0.98
(1,296)	1:21:A:ALA:HB3	1:56:A:GLN:HE21	34	0.98
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	13	0.97
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	12	0.96
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	2	0.95
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	28	0.93
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	11	0.92
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	33	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	19	0.91
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	20	0.91
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	3	0.89
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	8	0.89
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	21	0.89
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	22	0.89
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	14	0.88
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	39	0.88
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	23	0.87
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	38	0.87
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	7	0.86
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	18	0.86
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	29	0.86
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	35	0.85
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	6	0.82
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	9	0.82
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	26	0.82
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	27	0.82
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	1	0.81
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	15	0.81
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	17	0.8
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	24	0.8
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	25	0.8
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	32	0.8
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	40	0.8
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	10	0.79
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	31	0.79
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	5	0.78
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	16	0.78
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	36	0.77
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	30	0.76
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	37	0.76
(1,2090)	1:42:A:GLN:HA	1:42:A:GLN:HE21	4	0.75
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	3	0.62
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	3	0.62
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	3	0.62
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	3	0.62
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	3	0.62
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	3	0.62
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	1	0.5
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	1	0.5
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	1	0.5
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	1	0.5
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	1	0.5
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	1	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	33	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	33	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	33	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	33	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	33	0.5
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	14	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	14	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	33	0.5
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	33	0.5
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	33	0.5
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	30	0.5
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	30	0.5
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	30	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	30	0.5
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	17	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	17	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	17	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	17	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	17	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	17	0.49
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	17	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	2	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	2	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	2	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	2	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	2	0.49
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	2	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	25	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	25	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	25	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	25	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	25	0.49
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	25	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	20	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	20	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	27	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	27	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	27	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	27	0.49
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	27	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	27	0.49
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	27	0.49
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	35	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	35	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	35	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	35	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	35	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	35	0.48
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	35	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	25	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	25	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	36	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	36	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	36	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	36	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	36	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	36	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	36	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	40	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	40	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	40	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	40	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	40	0.48
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	40	0.48
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	40	0.48
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	24	0.47
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	24	0.47
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	24	0.47
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	24	0.47
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	24	0.47
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	24	0.47
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	24	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	29	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	29	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	30	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	30	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	30	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	30	0.47
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	30	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	30	0.47
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	30	0.47
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	3	0.47
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	3	0.47
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	3	0.47
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	18	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	40	0.46
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	39	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	39	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	39	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	39	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	39	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	39	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	14	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	14	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	14	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	14	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	14	0.45
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	14	0.45
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	32	0.45
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	32	0.45
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	32	0.45
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	32	0.45
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	32	0.45
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	32	0.45
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	30	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	30	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	30	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	30	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	30	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	30	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	34	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	34	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	34	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	34	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	34	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	34	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	6	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	13	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	13	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	13	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	13	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	13	0.44
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	13	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	21	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	21	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	39	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	39	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	39	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	39	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	39	0.44
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	39	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	39	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	39	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	39	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	39	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	39	0.44
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	39	0.44
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	27	0.43
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	27	0.43
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	27	0.43
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	27	0.43
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	27	0.43
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	27	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	33	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	34	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	34	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	34	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	34	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	34	0.43
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	34	0.43
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	4	0.43
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	4	0.43
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	4	0.43
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	4	0.43
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	4	0.43
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	4	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	34	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	34	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	34	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	34	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	34	0.43
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	34	0.43
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	34	0.43
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	34	0.43
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	34	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	34	0.43
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	31	0.41
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	31	0.41
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	31	0.41
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	31	0.41
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	31	0.41
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	31	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	32	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	32	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	32	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	32	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	32	0.41
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	32	0.41
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	32	0.41
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	18	0.41
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	18	0.41
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	18	0.41
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	40	0.41
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	40	0.41
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	40	0.41
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	6	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	21	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	32	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	32	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	32	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	32	0.4
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	32	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	32	0.4
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	29	0.4
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	29	0.4
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	29	0.4
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	29	0.4
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	29	0.4
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	29	0.4
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	6	0.4
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	38	0.4
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	38	0.4
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	38	0.4
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	38	0.4
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	38	0.4
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	38	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	12	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	12	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	12	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	12	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	12	0.4
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	12	0.4
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	12	0.4
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	33	0.4
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	33	0.4
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	33	0.4
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	33	0.4
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	33	0.4
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	33	0.4
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	33	0.4
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	33	0.4
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	33	0.4
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	33	0.4
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	33	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	33	0.4
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	7	0.4
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	7	0.4
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	7	0.4
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	21	0.4
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	21	0.4
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	21	0.4
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	8	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	21	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	22	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	22	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	22	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	22	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	22	0.39
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	22	0.39
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	7	0.39
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	13	0.39
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	16	0.39
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	16	0.39
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	16	0.39
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	16	0.39
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	16	0.39
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	40	0.39
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	40	0.39
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	40	0.39
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	29	0.39
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	29	0.39
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	29	0.39
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	32	0.38
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	32	0.38
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	32	0.38
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	32	0.38
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	32	0.38
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	32	0.38
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	32	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	7	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	31	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	31	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	31	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	31	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	31	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	31	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	37	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	40	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	40	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	40	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	40	0.38
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	40	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	40	0.38
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	34	0.38
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	34	0.38
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	34	0.38
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	34	0.38
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	34	0.38
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	34	0.38
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	17	0.38
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	17	0.38
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	17	0.38
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	17	0.38
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	17	0.38
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	17	0.38
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	17	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	30	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	30	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	30	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	40	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	40	0.38
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	40	0.38
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	20	0.37
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	20	0.37
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	20	0.37
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	20	0.37
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	20	0.37
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	20	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	4	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	24	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	24	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	24	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	24	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	24	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	24	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	29	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	29	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	29	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	29	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	29	0.37
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	29	0.37
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	32	0.37
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	32	0.37
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	32	0.37
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	32	0.37
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	32	0.37
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	32	0.37
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	15	0.37
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	26	0.37
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	26	0.37
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	26	0.37
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	26	0.37
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	26	0.37
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	26	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	35	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	35	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	35	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	35	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	35	0.37
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	35	0.37
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	35	0.37
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	12	0.37
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	12	0.37
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	12	0.37
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	25	0.37
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	25	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	25	0.37
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	15	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	15	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD11	22	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD12	22	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD13	22	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD21	22	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD22	22	0.36
(1,2817)	1:75:A:LYS:HB2	1:76:A:LEU:HD23	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD11	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD12	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD13	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD21	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD22	22	0.36
(1,2817)	1:75:A:LYS:HB3	1:76:A:LEU:HD23	22	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	25	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	25	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	25	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	25	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	25	0.36
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	25	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	2	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	2	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	2	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	2	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	2	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	2	0.36
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	19	0.36
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	19	0.36
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	19	0.36
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	19	0.36
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	19	0.36
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	37	0.36
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	37	0.36
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	37	0.36
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	37	0.36
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	37	0.36
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	37	0.36
(1,2364)	1:25:A:LEU:HD11	1:62:A:VAL:HA	7	0.36
(1,2364)	1:25:A:LEU:HD12	1:62:A:VAL:HA	7	0.36
(1,2364)	1:25:A:LEU:HD13	1:62:A:VAL:HA	7	0.36
(1,2364)	1:25:A:LEU:HD21	1:62:A:VAL:HA	7	0.36
(1,2364)	1:25:A:LEU:HD22	1:62:A:VAL:HA	7	0.36
(1,2364)	1:25:A:LEU:HD23	1:62:A:VAL:HA	7	0.36
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	18	0.36
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	22	0.36
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	22	0.36
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	22	0.36
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	22	0.36
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	22	0.36
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	22	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	2	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	2	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	2	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	2	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	2	0.36
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	2	0.36
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	2	0.36
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	25	0.36
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	25	0.36
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	25	0.36
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	36	0.36
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	36	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	36	0.36
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	26	0.35
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	26	0.35
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	26	0.35
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	26	0.35
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	26	0.35
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	26	0.35
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	24	0.35
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	24	0.35
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	24	0.35
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	24	0.35
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	24	0.35
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	24	0.35
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	19	0.35
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	19	0.35
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	19	0.35
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	19	0.35
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	19	0.35
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	19	0.35
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	29	0.35
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	29	0.35
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	29	0.35
(1,1462)	1:77:A:LEU:HD21	1:78:A:ASP:HA	39	0.35
(1,1462)	1:77:A:LEU:HD22	1:78:A:ASP:HA	39	0.35
(1,1462)	1:77:A:LEU:HD23	1:78:A:ASP:HA	39	0.35
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	21	0.35
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	21	0.35
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	21	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	14	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	14	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	14	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	31	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	31	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	31	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	33	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	33	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	33	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	39	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	39	0.35
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	39	0.35
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	19	0.34
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	19	0.34
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	19	0.34
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	19	0.34
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	19	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	20	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	20	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	20	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	20	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	20	0.34
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	20	0.34
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	6	0.34
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	23	0.34
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	28	0.34
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	38	0.34
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	38	0.34
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	38	0.34
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	38	0.34
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	38	0.34
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	38	0.34
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	40	0.34
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	40	0.34
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	40	0.34
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	40	0.34
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	40	0.34
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	40	0.34
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	40	0.34
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	40	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	40	0.34
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	39	0.34
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	39	0.34
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	39	0.34
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	27	0.34
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	27	0.34
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	27	0.34
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	2	0.34
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	2	0.34
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	2	0.34
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	17	0.33
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	17	0.33
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	17	0.33
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	17	0.33
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	17	0.33
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	17	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	35	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	35	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	35	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	35	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	35	0.33
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	35	0.33
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	21	0.33
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	21	0.33
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	21	0.33
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	21	0.33
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	21	0.33
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	21	0.33
(1,2236)	1:13:A:ASP:HB2	1:14:A:LYS:HG2	31	0.33
(1,2236)	1:13:A:ASP:HB2	1:14:A:LYS:HG3	31	0.33
(1,2236)	1:13:A:ASP:HB3	1:14:A:LYS:HG2	31	0.33
(1,2236)	1:13:A:ASP:HB3	1:14:A:LYS:HG3	31	0.33
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	31	0.33
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	31	0.33
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	31	0.33
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	33	0.33
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	33	0.33
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	33	0.33
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	32	0.33
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	32	0.33
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	32	0.33
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	30	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	30	0.33
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	30	0.33
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	36	0.32
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	36	0.32
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	36	0.32
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	36	0.32
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	36	0.32
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	36	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	4	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	24	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	24	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	24	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	24	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	24	0.32
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	24	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	1	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	12	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	12	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	12	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	12	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	12	0.32
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	12	0.32
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	5	0.32
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	22	0.32
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	22	0.32
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	22	0.32
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	22	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	22	0.32
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	22	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	23	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	23	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	37	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	37	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	37	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	37	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	37	0.32
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	37	0.32
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	37	0.32
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	27	0.32
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	27	0.32
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	40	0.32
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	40	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	40	0.32
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	40	0.32
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	40	0.32
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	40	0.32
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	40	0.32
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	34	0.32
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	34	0.32
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	34	0.32
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	7	0.32
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	7	0.32
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	7	0.32
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	18	0.32
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	18	0.32
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	18	0.32
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	30	0.32
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	30	0.32
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	30	0.32
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	32	0.32
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	32	0.32
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	32	0.32
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	32	0.32
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	32	0.32
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	32	0.32
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	33	0.32
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	33	0.32
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	33	0.32
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	6	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	6	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	6	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	6	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	6	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	6	0.31
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	6	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	11	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	11	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	11	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	11	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	11	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	28	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	31	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	31	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	31	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	31	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	31	0.31
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	31	0.31
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	31	0.31
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	14	0.31
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	14	0.31
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	14	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	6	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	6	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	6	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	6	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	6	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	6	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	24	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	24	0.31
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	24	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	24	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	24	0.31
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	24	0.31
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	20	0.31
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	20	0.31
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	20	0.31
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	25	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	25	0.31
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	25	0.31
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	36	0.31
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	36	0.31
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	36	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	7	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	7	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	7	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	20	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	20	0.31
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	20	0.31
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	14	0.31
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	14	0.31
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	14	0.31
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	39	0.31
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	39	0.31
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	39	0.31
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	19	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	19	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	37	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	37	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	37	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	37	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	37	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	37	0.3
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	37	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	12	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	12	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	12	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	12	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	12	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	36	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	38	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	38	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	38	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	38	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	38	0.3
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	38	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	9	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	15	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	18	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	18	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	18	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	18	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	18	0.3
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	18	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	25	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	25	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	25	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	25	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	25	0.3
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	25	0.3
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	32	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	32	0.3
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	32	0.3
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	32	0.3
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	32	0.3
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	32	0.3
(1,2364)	1:25:A:LEU:HD11	1:62:A:VAL:HA	24	0.3
(1,2364)	1:25:A:LEU:HD12	1:62:A:VAL:HA	24	0.3
(1,2364)	1:25:A:LEU:HD13	1:62:A:VAL:HA	24	0.3
(1,2364)	1:25:A:LEU:HD21	1:62:A:VAL:HA	24	0.3
(1,2364)	1:25:A:LEU:HD22	1:62:A:VAL:HA	24	0.3
(1,2364)	1:25:A:LEU:HD23	1:62:A:VAL:HA	24	0.3
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	21	0.3
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	25	0.3
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	31	0.3
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	31	0.3
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	31	0.3
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	31	0.3
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	31	0.3
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	31	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	24	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	24	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	24	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	24	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	24	0.3
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	24	0.3
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	24	0.3
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	20	0.3
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	20	0.3
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	20	0.3
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	20	0.3
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	20	0.3
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	20	0.3
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	20	0.3
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	20	0.3
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	20	0.3
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	20	0.3
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	20	0.3
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	39	0.3
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	39	0.3
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	39	0.3
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	23	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	23	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	24	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	24	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	24	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	24	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	24	0.29
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	24	0.29
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	24	0.29
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	29	0.29
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	29	0.29
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	29	0.29
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	29	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	29	0.29
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	29	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	17	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	17	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	17	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	17	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	17	0.29
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	17	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	29	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	29	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	29	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	29	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	29	0.29
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	29	0.29
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	39	0.29
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	39	0.29
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	39	0.29
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	39	0.29
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	39	0.29
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	39	0.29
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	36	0.29
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	36	0.29
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	36	0.29
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	36	0.29
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	36	0.29
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	36	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	17	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	17	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	17	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	17	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	17	0.29
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	17	0.29
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	17	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	21	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	21	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	21	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	30	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	30	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	30	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	32	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	32	0.29
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	32	0.29
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	36	0.29
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	36	0.29
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	36	0.29
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	36	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	19	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	19	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	19	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	19	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	19	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	19	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	22	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	22	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	22	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	22	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	22	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	22	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	23	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	23	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	23	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	23	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	23	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	23	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	37	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	37	0.29
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	37	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	37	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	37	0.29
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	37	0.29
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	21	0.29
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	21	0.29
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	21	0.29
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	4	0.29
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	4	0.29
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	4	0.29
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	15	0.29
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	15	0.29
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	15	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	15	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	15	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	15	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	15	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	15	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	7	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	32	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	32	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	32	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	32	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	32	0.28
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	32	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	30	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	30	0.28
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	30	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	32	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	36	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	36	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	36	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	36	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	36	0.28
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	36	0.28
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	25	0.28
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	25	0.28
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	25	0.28
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	25	0.28
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	25	0.28
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	25	0.28
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	24	0.28
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	24	0.28
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	24	0.28
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	24	0.28
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	24	0.28
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	24	0.28
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	24	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	36	0.28
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	36	0.28
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	36	0.28
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	28	0.28
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	28	0.28
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	28	0.28
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	28	0.28
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	28	0.28
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	28	0.28
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	4	0.28
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	4	0.28
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	4	0.28
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	27	0.28
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	27	0.28
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	27	0.28
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	18	0.28
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	18	0.28
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	18	0.28
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	18	0.28
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	18	0.28
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	18	0.28
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	27	0.28
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	27	0.28
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	27	0.28
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	28	0.27
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	28	0.27
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	28	0.27
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	28	0.27
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	28	0.27
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	28	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	5	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	30	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	30	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	30	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	30	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	30	0.27
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	30	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2478)	1:31:A:LEU:HD11	1:69:A:LEU:HG	11	0.27
(1,2478)	1:31:A:LEU:HD12	1:69:A:LEU:HG	11	0.27
(1,2478)	1:31:A:LEU:HD13	1:69:A:LEU:HG	11	0.27
(1,2478)	1:31:A:LEU:HD21	1:69:A:LEU:HG	11	0.27
(1,2478)	1:31:A:LEU:HD22	1:69:A:LEU:HG	11	0.27
(1,2478)	1:31:A:LEU:HD23	1:69:A:LEU:HG	11	0.27
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	18	0.27
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	29	0.27
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	29	0.27
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	29	0.27
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	29	0.27
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	29	0.27
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	29	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	28	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	28	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	28	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	28	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	28	0.27
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	28	0.27
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	28	0.27
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	25	0.27
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	25	0.27
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	25	0.27
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	18	0.27
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	18	0.27
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	18	0.27
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	2	0.27
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	2	0.27
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	2	0.27
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	34	0.27
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	34	0.27
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	34	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	27	0.27
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	27	0.27
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	27	0.27
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	27	0.27
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	27	0.27
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	27	0.27
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	4	0.27
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	4	0.27
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	4	0.27
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE1	14	0.27
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE2	14	0.27
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE3	14	0.27
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE1	14	0.27
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE2	14	0.27
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE3	14	0.27
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	40	0.26
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	40	0.26
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	40	0.26
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	40	0.26
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	40	0.26
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	40	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	5	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	5	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	28	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	28	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	28	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	28	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	28	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	28	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	28	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	28	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	28	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	28	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	28	0.26
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	28	0.26
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	14	0.26
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	14	0.26
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	14	0.26
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	14	0.26
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	14	0.26
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	14	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	26	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	35	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	35	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	35	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	35	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	35	0.26
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	35	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	19	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	38	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	38	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	38	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	38	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	38	0.26
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	38	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	14	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	14	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	14	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	14	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	14	0.26
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	14	0.26
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD11	40	0.26
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD12	40	0.26
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD13	40	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD21	40	0.26
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD22	40	0.26
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	14	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	14	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	18	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	18	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	40	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	40	0.26
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	40	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	31	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	31	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	31	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	31	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	31	0.26
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	31	0.26
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	30	0.26
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	30	0.26
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	30	0.26
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	30	0.26
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	30	0.26
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	30	0.26
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	14	0.26
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	14	0.26
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	14	0.26
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	14	0.26
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	14	0.26
(1,2297)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	11	0.26
(1,2297)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	11	0.26
(1,2297)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	11	0.26
(1,2297)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	11	0.26
(1,2297)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	11	0.26
(1,2297)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	11	0.26
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	40	0.26
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	40	0.26
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	40	0.26
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	5	0.26
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	5	0.26
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	5	0.26
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	5	0.26
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	5	0.26
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	5	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	25	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	25	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	25	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	34	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	34	0.26
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	34	0.26
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	24	0.26
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	24	0.26
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	24	0.26
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	6	0.26
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	6	0.26
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	6	0.26
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	14	0.26
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	14	0.26
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	14	0.26
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	14	0.26
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	14	0.26
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	14	0.26
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	20	0.26
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	20	0.26
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	20	0.26
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	36	0.26
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	36	0.26
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	36	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	19	0.26
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	19	0.26
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	19	0.26
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	38	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	38	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	38	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	38	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	38	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	38	0.25
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	38	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	39	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	39	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	39	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	39	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	39	0.25
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	39	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	20	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	20	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	27	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	27	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	27	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	27	0.25
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	27	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	7	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	7	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	7	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	7	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	7	0.25
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	7	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	5	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	5	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	18	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	18	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	18	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	18	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	18	0.25
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	18	0.25
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	18	0.25
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	27	0.25
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	27	0.25
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	27	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	33	0.25
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	33	0.25
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	33	0.25
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	25	0.25
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	25	0.25
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	25	0.25
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	20	0.25
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	20	0.25
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	20	0.25
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	36	0.25
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	36	0.25
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	36	0.25
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	38	0.25
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	38	0.25
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	38	0.25
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	38	0.25
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	38	0.25
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	38	0.25
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	6	0.25
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	6	0.25
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	6	0.25
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	31	0.25
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	31	0.25
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	31	0.25
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	34	0.25
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	34	0.25
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	34	0.25
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	29	0.25
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	29	0.25
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	29	0.25
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	25	0.25
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	25	0.25
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	25	0.25
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	12	0.25
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	12	0.25
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	12	0.25
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	34	0.25
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	34	0.25
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	34	0.25
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE1	31	0.25
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE2	31	0.25
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE3	31	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE1	31	0.25
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE2	31	0.25
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE3	31	0.25
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	11	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	11	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD11	22	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD12	22	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD13	22	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD21	22	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD22	22	0.24
(1,2770)	1:68:A:SER:HB2	1:69:A:LEU:HD23	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD11	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD12	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD13	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD21	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD22	22	0.24
(1,2770)	1:68:A:SER:HB3	1:69:A:LEU:HD23	22	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	16	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	23	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	23	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	23	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	23	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	23	0.24
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	23	0.24
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	34	0.24
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	34	0.24
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	34	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	34	0.24
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	34	0.24
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	34	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	12	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	33	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	33	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	33	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	33	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	33	0.24
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	33	0.24
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	34	0.24
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	34	0.24
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	34	0.24
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	34	0.24
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	34	0.24
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	34	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	8	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	8	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	31	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	31	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	31	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	31	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	31	0.24
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	31	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	31	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	31	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	31	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	31	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	31	0.24
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	31	0.24
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	31	0.24
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	31	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	29	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	29	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	29	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	29	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	29	0.24
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	29	0.24
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	33	0.24
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	33	0.24
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	33	0.24
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	37	0.24
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	37	0.24
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	37	0.24
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	17	0.24
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	17	0.24
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	17	0.24
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	37	0.24
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	37	0.24
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	37	0.24
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	29	0.24
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	29	0.24
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	29	0.24
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	29	0.24
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	29	0.24
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	29	0.24
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	40	0.24
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	40	0.24
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	40	0.24
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	29	0.24
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	29	0.24
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	29	0.24
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	39	0.24
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	39	0.24
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	39	0.24
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	1	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	1	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	1	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	1	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	1	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	5	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	23	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	23	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	23	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	23	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	23	0.23
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	23	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	36	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	36	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	36	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	36	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	36	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	36	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	20	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	20	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	20	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	20	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	20	0.23
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	20	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	31	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	31	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	31	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	31	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	31	0.23
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	31	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	4	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	31	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	31	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	31	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	31	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	31	0.23
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	31	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	6	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	33	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	33	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	33	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	33	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	33	0.23
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	33	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD11	20	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD12	20	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD13	20	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD21	20	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD22	20	0.23
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD23	20	0.23
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	27	0.23
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	32	0.23
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	32	0.23
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	32	0.23
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	32	0.23
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	32	0.23
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	32	0.23
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	34	0.23
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	34	0.23
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	34	0.23
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	29	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	14	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	14	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	14	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	20	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	20	0.23
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD11	20	0.23
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD12	20	0.23
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD13	20	0.23
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	31	0.23
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	31	0.23
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	31	0.23
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	31	0.23
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	21	0.23
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	21	0.23
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	21	0.23
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	14	0.23
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	14	0.23
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	14	0.23
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	27	0.23
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	27	0.23
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	27	0.23
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	30	0.23
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	30	0.23
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	30	0.23
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	31	0.23
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	31	0.23
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	31	0.23
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	17	0.23
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	17	0.23
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	17	0.23
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	24	0.23
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	24	0.23
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	24	0.23
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	18	0.23
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	18	0.23
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	18	0.23
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	19	0.23
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	19	0.23
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	19	0.23
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	1	0.23
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	1	0.23
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	1	0.23
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	24	0.23
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	24	0.23
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	24	0.23
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	29	0.23
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	29	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	29	0.23
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	21	0.23
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	21	0.23
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	21	0.23
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	40	0.23
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	40	0.23
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	40	0.23
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	27	0.22
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	27	0.22
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	27	0.22
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	27	0.22
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	27	0.22
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	27	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	21	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	21	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	21	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	21	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	21	0.22
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	21	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	33	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	33	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	33	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	33	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	33	0.22
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	33	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	36	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	36	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	36	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	36	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	36	0.22
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	36	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	12	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	24	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	24	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	24	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	24	0.22
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	24	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	24	0.22
(1,2364)	1:25:A:LEU:HD11	1:62:A:VAL:HA	5	0.22
(1,2364)	1:25:A:LEU:HD12	1:62:A:VAL:HA	5	0.22
(1,2364)	1:25:A:LEU:HD13	1:62:A:VAL:HA	5	0.22
(1,2364)	1:25:A:LEU:HD21	1:62:A:VAL:HA	5	0.22
(1,2364)	1:25:A:LEU:HD22	1:62:A:VAL:HA	5	0.22
(1,2364)	1:25:A:LEU:HD23	1:62:A:VAL:HA	5	0.22
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	30	0.22
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	30	0.22
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	30	0.22
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	30	0.22
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	30	0.22
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	30	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	20	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	20	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	20	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	20	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	20	0.22
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	20	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	40	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	40	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	40	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	40	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	40	0.22
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	40	0.22
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	13	0.22
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	13	0.22
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	13	0.22
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	29	0.22
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	29	0.22
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	29	0.22
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	19	0.22
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	19	0.22
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	19	0.22
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	19	0.22
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	29	0.22
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	29	0.22
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	29	0.22
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	29	0.22
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	29	0.22
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	12	0.22
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	12	0.22
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	19	0.22
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	19	0.22
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	19	0.22
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	23	0.22
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	23	0.22
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	23	0.22
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	30	0.22
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	30	0.22
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	30	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	17	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	17	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	17	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	24	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	24	0.22
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	24	0.22
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	25	0.22
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	25	0.22
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	25	0.22
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	30	0.22
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	30	0.22
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	30	0.22
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	34	0.22
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	34	0.22
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	34	0.22
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	34	0.22
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	34	0.22
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	34	0.22
(1,468)	1:32:A:LYS:HG2	1:65:A:LEU:HD11	6	0.22
(1,468)	1:32:A:LYS:HG2	1:65:A:LEU:HD12	6	0.22
(1,468)	1:32:A:LYS:HG2	1:65:A:LEU:HD13	6	0.22
(1,468)	1:32:A:LYS:HG3	1:65:A:LEU:HD11	6	0.22
(1,468)	1:32:A:LYS:HG3	1:65:A:LEU:HD12	6	0.22
(1,468)	1:32:A:LYS:HG3	1:65:A:LEU:HD13	6	0.22
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	40	0.22
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	40	0.22
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	40	0.22
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	34	0.22
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	34	0.22
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	34	0.22
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	26	0.22
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	26	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	26	0.22
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	40	0.21
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	40	0.21
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	40	0.21
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	40	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	22	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	22	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	22	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	22	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	22	0.21
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	22	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	10	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	10	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	10	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	10	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	10	0.21
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	10	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	20	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	20	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	20	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	20	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	20	0.21
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	20	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	36	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	36	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	36	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	36	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	36	0.21
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	29	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	36	0.21
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	36	0.21
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	4	0.21
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	4	0.21
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	4	0.21
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	4	0.21
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	4	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	9	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	9	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	9	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	9	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	9	0.21
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	9	0.21
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	9	0.21
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	34	0.21
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	21	0.21
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	21	0.21
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	21	0.21
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	40	0.21
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	40	0.21
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	40	0.21
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD11	11	0.21
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD12	11	0.21
(1,1115)	1:68:A:SER:HB2	1:69:A:LEU:HD13	11	0.21
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD11	11	0.21
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD12	11	0.21
(1,1115)	1:68:A:SER:HB3	1:69:A:LEU:HD13	11	0.21
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	36	0.21
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	36	0.21
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	36	0.21
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	6	0.21
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	6	0.21
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	6	0.21
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	21	0.21
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	21	0.21
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	21	0.21
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	25	0.21
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	25	0.21
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	25	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	40	0.21
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	40	0.21
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	40	0.21
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	25	0.21
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	25	0.21
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	25	0.21
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	30	0.21
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	30	0.21
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	30	0.21
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	34	0.21
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	34	0.21
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	34	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	2	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	2	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	2	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	16	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	16	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	16	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	23	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	23	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	23	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	26	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	26	0.21
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	26	0.21
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	30	0.21
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	30	0.21
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	30	0.21
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	30	0.21
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	30	0.21
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	30	0.21
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	34	0.21
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	34	0.21
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	34	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	25	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	25	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	25	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	31	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	31	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	31	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	33	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	33	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	33	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	36	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	36	0.21
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	36	0.21
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	6	0.21
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	6	0.21
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	6	0.21
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	13	0.21
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	13	0.21
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	13	0.21
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	18	0.21
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	18	0.21
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	18	0.21
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	18	0.21
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	18	0.21
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	18	0.21
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	21	0.21
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	21	0.21
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	21	0.21
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	29	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	32	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	32	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	32	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	32	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	32	0.2
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	32	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	9	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	11	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	11	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	11	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	11	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	11	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	13	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	13	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	13	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	13	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	13	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	13	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	4	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	21	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	40	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	40	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	40	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	40	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	40	0.2
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	40	0.2
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	29	0.2
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	29	0.2
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	29	0.2
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	29	0.2
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	29	0.2
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	25	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	29	0.2
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	29	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	14	0.2
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	14	0.2
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	14	0.2
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	14	0.2
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	14	0.2
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	14	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	31	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	31	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	31	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	31	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	31	0.2
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	31	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	39	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	39	0.2
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	39	0.2
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	39	0.2
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	39	0.2
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	39	0.2
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	39	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	25	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	25	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	25	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	25	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	25	0.2
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	25	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	7	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	17	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	17	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	17	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	17	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	17	0.2
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	17	0.2
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	24	0.2
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	35	0.2
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	35	0.2
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	35	0.2
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	35	0.2
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	35	0.2
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	35	0.2
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	27	0.2
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	27	0.2
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	27	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	27	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	27	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	27	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	31	0.2
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	31	0.2
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	31	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	31	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	31	0.2
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	31	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	1	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	1	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	7	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	7	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	7	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	7	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	7	0.2
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	7	0.2
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	7	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	30	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	30	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	30	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	30	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	30	0.2
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	30	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	34	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	34	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	34	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	34	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	34	0.2
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	34	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	30	0.2
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	30	0.2
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	30	0.2
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	25	0.2
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	30	0.2
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	39	0.2
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	39	0.2
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	39	0.2
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	39	0.2
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	39	0.2
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	39	0.2
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	39	0.2
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	39	0.2
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	21	0.2
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	21	0.2
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	21	0.2
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	25	0.2
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	25	0.2
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	25	0.2
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	40	0.2
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	40	0.2
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	40	0.2
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	5	0.2
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	5	0.2
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	5	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	25	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	25	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	25	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	29	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	29	0.2
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	29	0.2
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	34	0.2
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	34	0.2
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	34	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	29	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	29	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	29	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	40	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	40	0.2
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	40	0.2
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	5	0.2
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	5	0.2
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	39	0.2
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	39	0.2
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	39	0.2
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	39	0.2
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	39	0.2
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	39	0.2
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	30	0.2
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	30	0.2
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	30	0.2
(1,439)	1:25:A:LEU:HD11	1:62:A:VAL:H	39	0.2
(1,439)	1:25:A:LEU:HD12	1:62:A:VAL:H	39	0.2
(1,439)	1:25:A:LEU:HD13	1:62:A:VAL:H	39	0.2
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	31	0.2
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	31	0.2
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	31	0.2
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	38	0.2
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	38	0.2
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	38	0.2
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	4	0.2
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	4	0.2
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	4	0.2
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	36	0.2
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	36	0.2
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	36	0.2
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	16	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	16	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	16	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	16	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	16	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	16	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	2	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	19	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	19	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	19	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	19	0.19
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	19	0.19
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	18	0.19
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	18	0.19
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	18	0.19
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	18	0.19
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	18	0.19
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	7	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	18	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	27	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	30	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	32	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	33	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	33	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	33	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	33	0.19
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	33	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	33	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	40	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	40	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	40	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	40	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	40	0.19
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	40	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	32	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	32	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	32	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	32	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	32	0.19
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	32	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	20	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	27	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	30	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	39	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	39	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	39	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	39	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	39	0.19
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	39	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	2	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	2	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	2	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	2	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	2	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	37	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	37	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	37	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	37	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	37	0.19
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	37	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	24	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	24	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	24	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	24	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	24	0.19
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	24	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD11	17	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD12	17	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD13	17	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD21	17	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD22	17	0.19
(1,2391)	1:27:A:LEU:HG	1:28:A:LEU:HD23	17	0.19
(1,2357)	1:25:A:LEU:HD11	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD11	1:29:A:LYS:HE3	1	0.19
(1,2357)	1:25:A:LEU:HD12	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD12	1:29:A:LYS:HE3	1	0.19
(1,2357)	1:25:A:LEU:HD13	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD13	1:29:A:LYS:HE3	1	0.19
(1,2357)	1:25:A:LEU:HD21	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD21	1:29:A:LYS:HE3	1	0.19
(1,2357)	1:25:A:LEU:HD22	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD22	1:29:A:LYS:HE3	1	0.19
(1,2357)	1:25:A:LEU:HD23	1:29:A:LYS:HE2	1	0.19
(1,2357)	1:25:A:LEU:HD23	1:29:A:LYS:HE3	1	0.19
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	4	0.19
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	12	0.19
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	12	0.19
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	12	0.19
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	12	0.19
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	12	0.19
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	21	0.19
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	21	0.19
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	21	0.19
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	21	0.19
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	21	0.19
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	21	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	19	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	19	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	19	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	19	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	19	0.19
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	19	0.19
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	19	0.19
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	18	0.19
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	18	0.19
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	32	0.19
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	12	0.19
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	12	0.19
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	12	0.19
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	25	0.19
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	25	0.19
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	25	0.19
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD2	31	0.19
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD3	31	0.19
(1,1462)	1:77:A:LEU:HD21	1:78:A:ASP:HA	15	0.19
(1,1462)	1:77:A:LEU:HD22	1:78:A:ASP:HA	15	0.19
(1,1462)	1:77:A:LEU:HD23	1:78:A:ASP:HA	15	0.19
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	4	0.19
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	4	0.19
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	4	0.19
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	34	0.19
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	34	0.19
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	34	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	27	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	27	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	27	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	31	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	31	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	31	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	33	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	33	0.19
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	33	0.19
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	39	0.19
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	39	0.19
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	39	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	30	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	30	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	30	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	31	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	31	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	31	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	33	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	33	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	33	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	39	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	39	0.19
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	39	0.19
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	14	0.19
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	14	0.19
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	14	0.19
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	39	0.19
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	39	0.19
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	39	0.19
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	25	0.19
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	25	0.19
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	25	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	15	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	15	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	15	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	28	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	28	0.19
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	28	0.19
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	6	0.19
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	6	0.19
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	6	0.19
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	20	0.19
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	20	0.19
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	20	0.19
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	20	0.19
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	20	0.19
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	21	0.19
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	21	0.19
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	21	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	14	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	14	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	14	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	21	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	21	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	21	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	29	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	29	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	29	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	39	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	39	0.19
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	39	0.19
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	40	0.19
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	40	0.19
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	40	0.19
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	23	0.19
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	23	0.19
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	23	0.19
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	37	0.19
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	37	0.19
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	37	0.19
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	11	0.19
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	11	0.19
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	11	0.19
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	25	0.19
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	25	0.19
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	25	0.19
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	32	0.19
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	32	0.19
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	32	0.19
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	37	0.18
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	37	0.18
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	37	0.18
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	37	0.18
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	37	0.18
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	37	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	30	0.18
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	30	0.18
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	30	0.18
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	30	0.18
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	30	0.18
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	30	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	39	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	39	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	39	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	39	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	39	0.18
(1,2613)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	39	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	18	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	18	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	18	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	18	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	18	0.18
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	18	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	14	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	14	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	14	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	14	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	14	0.18
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	14	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	25	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	29	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	29	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	29	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	29	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	29	0.18
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	29	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	7	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	7	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	7	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	7	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	7	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	18	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	19	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	21	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	32	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	32	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	32	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	32	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	32	0.18
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	32	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	22	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	23	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	26	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	26	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	26	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	26	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	26	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	26	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	35	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	35	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	35	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	35	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	35	0.18
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	35	0.18
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	22	0.18
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	22	0.18
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	22	0.18
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	22	0.18
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	22	0.18
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	22	0.18
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	33	0.18
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	33	0.18
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	33	0.18
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	33	0.18
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	33	0.18
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	33	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD11	7	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD12	7	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD13	7	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD21	7	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD22	7	0.18
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD23	7	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	18	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	18	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	18	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	18	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	18	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	18	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	39	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	39	0.18
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	39	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	39	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	39	0.18
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	39	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	4	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	4	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	4	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	4	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	4	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	4	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	15	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	15	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	16	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	16	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	16	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	16	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	16	0.18
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	16	0.18
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	16	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	18	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	18	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	18	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	18	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	18	0.18
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	18	0.18
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	32	0.18
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	32	0.18
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	32	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	32	0.18
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	32	0.18
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	32	0.18
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	32	0.18
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	40	0.18
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	40	0.18
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	40	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	6	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	6	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	6	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	14	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	14	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	14	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	36	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	36	0.18
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	36	0.18
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	20	0.18
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	20	0.18
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	20	0.18
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	7	0.18
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	7	0.18
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	7	0.18
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	39	0.18
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	39	0.18
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	39	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	14	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	14	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	14	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	20	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	20	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	20	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	39	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	39	0.18
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	39	0.18
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG21	23	0.18
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG22	23	0.18
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG23	23	0.18
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG21	23	0.18
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG22	23	0.18
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG23	23	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	38	0.18
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	38	0.18
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	38	0.18
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	5	0.18
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	5	0.18
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	5	0.18
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	15	0.18
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	15	0.18
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	15	0.18
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	26	0.18
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	26	0.18
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	26	0.18
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	35	0.18
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	35	0.18
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	35	0.18
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	20	0.18
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	20	0.18
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	20	0.18
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	27	0.18
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	27	0.18
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	27	0.18
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	29	0.18
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	29	0.18
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	29	0.18
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	34	0.18
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	34	0.18
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	34	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	18	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	18	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	18	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	31	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	31	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	31	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	36	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	36	0.18
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	36	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	22	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	22	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	22	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	35	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	35	0.18
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	35	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	16	0.18
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	16	0.18
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	16	0.18
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	40	0.18
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	40	0.18
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	40	0.18
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	40	0.18
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	40	0.18
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	40	0.18
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	14	0.18
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	14	0.18
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	14	0.18
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	18	0.18
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	18	0.18
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	18	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	18	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	18	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	18	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	27	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	27	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	27	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	32	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	32	0.18
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	32	0.18
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	18	0.18
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	18	0.18
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	18	0.18
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	16	0.18
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	16	0.18
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	16	0.18
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	22	0.18
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	22	0.18
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	22	0.18
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	25	0.18
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	25	0.18
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	25	0.18
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	31	0.18
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	31	0.18
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	31	0.18
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD11	27	0.17
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD12	27	0.17
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD13	27	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD21	27	0.17
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD22	27	0.17
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD23	27	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	10	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	10	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	10	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	10	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	10	0.17
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	10	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	30	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	30	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	30	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	30	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	30	0.17
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	30	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	36	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	36	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	36	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	36	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	36	0.17
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	36	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	39	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	39	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	39	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	39	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	39	0.17
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	39	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	40	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	40	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	40	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	40	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	40	0.17
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	18	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	21	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	21	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	21	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	21	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	21	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	21	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	29	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	36	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	39	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	40	0.17
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	40	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	15	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	15	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	15	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	15	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	15	0.17
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	15	0.17
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	13	0.17
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	28	0.17
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	28	0.17
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	28	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	28	0.17
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	28	0.17
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	28	0.17
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	19	0.17
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	19	0.17
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	19	0.17
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	19	0.17
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	19	0.17
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	19	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	14	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	14	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	14	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	14	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	14	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	14	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	25	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	25	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	25	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	25	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	25	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	25	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	32	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	32	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	32	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	32	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	32	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	32	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	33	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	33	0.17
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	33	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	33	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	33	0.17
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	33	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	3	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	3	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	3	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	3	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	3	0.17
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	3	0.17
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	3	0.17
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	3	0.17
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	3	0.17
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	3	0.17
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	3	0.17
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	25	0.17
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	25	0.17
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	25	0.17
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	37	0.17
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	37	0.17
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	37	0.17
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD11	30	0.17
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD12	30	0.17
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD13	30	0.17
(1,1462)	1:77:A:LEU:HD21	1:78:A:ASP:HA	26	0.17
(1,1462)	1:77:A:LEU:HD22	1:78:A:ASP:HA	26	0.17
(1,1462)	1:77:A:LEU:HD23	1:78:A:ASP:HA	26	0.17
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	38	0.17
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	38	0.17
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	38	0.17
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	38	0.17
(1,1342)	1:41:A:LEU:HA	1:103:A:LEU:HD11	34	0.17
(1,1342)	1:41:A:LEU:HA	1:103:A:LEU:HD12	34	0.17
(1,1342)	1:41:A:LEU:HA	1:103:A:LEU:HD13	34	0.17
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	18	0.17
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	18	0.17
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	18	0.17
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	24	0.17
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	24	0.17
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	25	0.17
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	31	0.17
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	32	0.17
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	30	0.17
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	30	0.17
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	30	0.17
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG21	7	0.17
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG22	7	0.17
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG23	7	0.17
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG21	7	0.17
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG22	7	0.17
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG23	7	0.17
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	28	0.17
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	28	0.17
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	28	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	37	0.17
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	37	0.17
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	37	0.17
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	38	0.17
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	38	0.17
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	38	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	36	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	36	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	36	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	40	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	40	0.17
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	40	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	30	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	30	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	30	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	36	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	36	0.17
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	36	0.17
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	30	0.17
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	30	0.17
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	30	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	1	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	1	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	1	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	38	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	38	0.17
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	38	0.17
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	40	0.17
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	40	0.17
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	40	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	25	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	25	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	25	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	25	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	25	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	25	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	26	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	26	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	26	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	26	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	26	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	26	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	33	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	33	0.17
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	33	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	33	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	33	0.17
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	33	0.17
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	27	0.17
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	27	0.17
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	27	0.17
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	4	0.17
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	4	0.17
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	4	0.17
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	34	0.17
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	34	0.17
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	34	0.17
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	1	0.17
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	1	0.17
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	1	0.17
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	17	0.17
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	17	0.17
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	17	0.17
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	35	0.17
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	35	0.17
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	35	0.17
(1,259)	1:16:A:VAL:HG11	1:56:A:GLN:HE21	7	0.17
(1,259)	1:16:A:VAL:HG12	1:56:A:GLN:HE21	7	0.17
(1,259)	1:16:A:VAL:HG13	1:56:A:GLN:HE21	7	0.17
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	18	0.17
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	18	0.17
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	18	0.17
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	18	0.17
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	18	0.17
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	18	0.17
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	18	0.17
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	18	0.17
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	18	0.17
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	20	0.17
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	20	0.17
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	20	0.17
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	30	0.17
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	30	0.17
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	30	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	34	0.17
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	34	0.17
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	34	0.17
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	36	0.17
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	36	0.17
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	36	0.17
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	29	0.17
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	29	0.17
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	29	0.17
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	30	0.17
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	30	0.17
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	30	0.17
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	32	0.17
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	32	0.17
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	32	0.17
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	33	0.17
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	33	0.17
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	33	0.17
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	18	0.16
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	18	0.16
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	18	0.16
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	18	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	12	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	27	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	27	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	27	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	27	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	27	0.16
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	27	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	8	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	8	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	8	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	8	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	8	0.16
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	8	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	7	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	7	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	7	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	7	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	7	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	24	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	32	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	33	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	33	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	33	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	33	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	33	0.16
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	33	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	6	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	31	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	39	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	39	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	39	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	39	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	39	0.16
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	39	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	25	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	25	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	25	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	25	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	25	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	25	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	34	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	34	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	34	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	34	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	34	0.16
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	34	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	14	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	20	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	20	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	20	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	20	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	20	0.16
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	20	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	16	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	16	0.16
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	16	0.16
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	16	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	19	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	19	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	19	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	19	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	19	0.16
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	19	0.16
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	36	0.16
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	36	0.16
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	36	0.16
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	36	0.16
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	36	0.16
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	36	0.16
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	7	0.16
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	7	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	4	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	14	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	14	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	14	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	14	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	14	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	25	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	27	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	36	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	39	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	39	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	39	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	39	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	39	0.16
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	39	0.16
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	21	0.16
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	21	0.16
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	21	0.16
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	2	0.16
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	2	0.16
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	2	0.16
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	19	0.16
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	19	0.16
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	19	0.16
(1,1482)	1:32:A:LYS:HE2	1:65:A:LEU:HD11	7	0.16
(1,1482)	1:32:A:LYS:HE2	1:65:A:LEU:HD12	7	0.16
(1,1482)	1:32:A:LYS:HE2	1:65:A:LEU:HD13	7	0.16
(1,1482)	1:32:A:LYS:HE3	1:65:A:LEU:HD11	7	0.16
(1,1482)	1:32:A:LYS:HE3	1:65:A:LEU:HD12	7	0.16
(1,1482)	1:32:A:LYS:HE3	1:65:A:LEU:HD13	7	0.16
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	29	0.16
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	29	0.16
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	29	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	4	0.16
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	4	0.16
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	4	0.16
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	4	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	6	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	6	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	6	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	31	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	31	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	31	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	36	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	36	0.16
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	36	0.16
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	17	0.16
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	17	0.16
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	12	0.16
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	12	0.16
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	12	0.16
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	30	0.16
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	32	0.16
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	32	0.16
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	32	0.16
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	40	0.16
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	40	0.16
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	40	0.16
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	1	0.16
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	1	0.16
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	1	0.16
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	9	0.16
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	9	0.16
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	9	0.16
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	22	0.16
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	22	0.16
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	22	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	4	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	4	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	4	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	34	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	34	0.16
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	34	0.16
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	40	0.16
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	40	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	40	0.16
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	39	0.16
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	39	0.16
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	39	0.16
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	21	0.16
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	21	0.16
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	21	0.16
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	11	0.16
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	11	0.16
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	11	0.16
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	39	0.16
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	39	0.16
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	39	0.16
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	7	0.16
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	7	0.16
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	7	0.16
(1,324)	1:24:A:ALA:HB1	1:62:A:VAL:HB	40	0.16
(1,324)	1:24:A:ALA:HB2	1:62:A:VAL:HB	40	0.16
(1,324)	1:24:A:ALA:HB3	1:62:A:VAL:HB	40	0.16
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	30	0.16
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	30	0.16
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	30	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	20	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	20	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	20	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	20	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	20	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	20	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	20	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	20	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	20	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	39	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	39	0.16
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	39	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	39	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	39	0.16
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	39	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	39	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	39	0.16
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	39	0.16
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	29	0.16
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	29	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	29	0.16
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	7	0.16
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	7	0.16
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	7	0.16
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	27	0.16
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	27	0.16
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	27	0.16
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	7	0.15
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	7	0.15
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	7	0.15
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	7	0.15
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	29	0.15
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	29	0.15
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	29	0.15
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	29	0.15
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	29	0.15
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	29	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	33	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	33	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	33	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	33	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	33	0.15
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	33	0.15
(1,2725)	1:59:A:ASP:HB2	1:62:A:VAL:HB	29	0.15
(1,2725)	1:59:A:ASP:HB3	1:62:A:VAL:HB	29	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	13	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	15	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	15	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	15	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	15	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	15	0.15
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	15	0.15
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	31	0.15
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	31	0.15
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	31	0.15
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	31	0.15
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	31	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	31	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	4	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	22	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	22	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	22	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	22	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	22	0.15
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	22	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	7	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	27	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	32	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	34	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	34	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	34	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	34	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	34	0.15
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	34	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	34	0.15
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	34	0.15
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	34	0.15
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	34	0.15
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	34	0.15
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	34	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	2	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	2	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	2	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	2	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	2	0.15
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	2	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	5	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	5	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	5	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	5	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	5	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	38	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	38	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	38	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	38	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	38	0.15
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	38	0.15
(1,2437)	1:29:A:LYS:H	1:29:A:LYS:HG2	1	0.15
(1,2437)	1:29:A:LYS:H	1:29:A:LYS:HG3	1	0.15
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	8	0.15
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	9	0.15
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	11	0.15
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	11	0.15
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	11	0.15
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	11	0.15
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	11	0.15
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	11	0.15
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	6	0.15
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	6	0.15
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	6	0.15
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	6	0.15
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	6	0.15
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	6	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD11	40	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD12	40	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD13	40	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD21	40	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD22	40	0.15
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD23	40	0.15
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB2	34	0.15
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB3	34	0.15
(1,2362)	1:25:A:LEU:HD11	1:61:A:GLU:HG2	30	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2362)	1:25:A:LEU:HD11	1:61:A:GLU:HG3	30	0.15
(1,2362)	1:25:A:LEU:HD12	1:61:A:GLU:HG2	30	0.15
(1,2362)	1:25:A:LEU:HD12	1:61:A:GLU:HG3	30	0.15
(1,2362)	1:25:A:LEU:HD13	1:61:A:GLU:HG2	30	0.15
(1,2362)	1:25:A:LEU:HD13	1:61:A:GLU:HG3	30	0.15
(1,2362)	1:25:A:LEU:HD21	1:61:A:GLU:HG2	30	0.15
(1,2362)	1:25:A:LEU:HD21	1:61:A:GLU:HG3	30	0.15
(1,2362)	1:25:A:LEU:HD22	1:61:A:GLU:HG2	30	0.15
(1,2362)	1:25:A:LEU:HD22	1:61:A:GLU:HG3	30	0.15
(1,2362)	1:25:A:LEU:HD23	1:61:A:GLU:HG2	30	0.15
(1,2362)	1:25:A:LEU:HD23	1:61:A:GLU:HG3	30	0.15
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	5	0.15
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	5	0.15
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	5	0.15
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	5	0.15
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	5	0.15
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	5	0.15
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	23	0.15
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	37	0.15
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	37	0.15
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	37	0.15
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	37	0.15
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	37	0.15
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	37	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD11	21	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD12	21	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD13	21	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD21	21	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD22	21	0.15
(1,2349)	1:25:A:LEU:HB3	1:28:A:LEU:HD23	21	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD11	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD12	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD13	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD21	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD22	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD23	5	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD11	24	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD12	24	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD13	24	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD21	24	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD22	24	0.15
(1,2340)	1:25:A:LEU:HA	1:25:A:LEU:HD23	24	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	4	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	4	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	4	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	4	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	4	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	4	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	6	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	6	0.15
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	6	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	6	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	6	0.15
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	6	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	6	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	10	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	10	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	10	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	10	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	10	0.15
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	10	0.15
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	10	0.15
(1,1896)	1:59:A:ASP:H	1:62:A:VAL:HB	29	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	18	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	18	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	18	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	27	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	27	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	27	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	39	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	39	0.15
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	39	0.15
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	24	0.15
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	24	0.15
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	24	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	4	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	4	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	4	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	6	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	6	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	6	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	24	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	24	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	24	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	28	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	28	0.15
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	28	0.15
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	7	0.15
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	7	0.15
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	7	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	7	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	7	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	7	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	14	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	14	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	14	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	27	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	27	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	27	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	33	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	33	0.15
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	33	0.15
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	34	0.15
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	4	0.15
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	4	0.15
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	12	0.15
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	12	0.15
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	12	0.15
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	13	0.15
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	13	0.15
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	13	0.15
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	30	0.15
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	30	0.15
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	30	0.15
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	21	0.15
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	21	0.15
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	21	0.15
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	32	0.15
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	32	0.15
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	32	0.15
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	36	0.15
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	36	0.15
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	36	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	25	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	25	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	25	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	32	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	32	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	32	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	33	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	33	0.15
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	33	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	31	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	31	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	31	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	33	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	33	0.15
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	33	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	4	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	4	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	4	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	30	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	30	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	30	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	32	0.15
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	32	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	32	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	8	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	8	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	8	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	9	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	9	0.15
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	9	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	21	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	21	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	21	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	21	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	21	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	21	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	24	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	24	0.15
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	24	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	24	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	24	0.15
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	24	0.15
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	20	0.15
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	20	0.15
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	20	0.15
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD11	32	0.15
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD12	32	0.15
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD13	32	0.15
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD11	32	0.15
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD12	32	0.15
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD13	32	0.15
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	20	0.15
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	20	0.15
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	20	0.15
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	27	0.15
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	27	0.15
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	27	0.15
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	27	0.15
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	27	0.15
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	27	0.15
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	27	0.15
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	27	0.15
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	27	0.15
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	25	0.15
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	25	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	25	0.15
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	31	0.15
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	31	0.15
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	31	0.15
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	2	0.15
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	2	0.15
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	2	0.15
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	20	0.15
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	20	0.15
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	20	0.15
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	23	0.15
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	23	0.15
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	23	0.15
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	21	0.14
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	21	0.14
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	21	0.14
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	21	0.14
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	21	0.14
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	21	0.14
(1,2844)	1:77:A:LEU:HD11	1:103:A:LEU:H	39	0.14
(1,2844)	1:77:A:LEU:HD12	1:103:A:LEU:H	39	0.14
(1,2844)	1:77:A:LEU:HD13	1:103:A:LEU:H	39	0.14
(1,2844)	1:77:A:LEU:HD21	1:103:A:LEU:H	39	0.14
(1,2844)	1:77:A:LEU:HD22	1:103:A:LEU:H	39	0.14
(1,2844)	1:77:A:LEU:HD23	1:103:A:LEU:H	39	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	4	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	4	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	4	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	4	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	4	0.14
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	4	0.14
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	4	0.14
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	30	0.14
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	30	0.14
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	30	0.14
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	30	0.14
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	30	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	30	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	39	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	39	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	39	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	39	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	39	0.14
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	39	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	12	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	22	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	36	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	36	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	36	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	36	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	36	0.14
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	36	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	17	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	19	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	19	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	19	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	19	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	19	0.14
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	19	0.14
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	24	0.14
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	24	0.14
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	24	0.14
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	24	0.14
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	24	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	24	0.14
(1,2517)	1:37:A:THR:HG21	1:39:A:GLU:HB2	15	0.14
(1,2517)	1:37:A:THR:HG21	1:39:A:GLU:HB3	15	0.14
(1,2517)	1:37:A:THR:HG22	1:39:A:GLU:HB2	15	0.14
(1,2517)	1:37:A:THR:HG22	1:39:A:GLU:HB3	15	0.14
(1,2517)	1:37:A:THR:HG23	1:39:A:GLU:HB2	15	0.14
(1,2517)	1:37:A:THR:HG23	1:39:A:GLU:HB3	15	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	19	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	33	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	33	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	33	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	33	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	33	0.14
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	33	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG22	30	0.14
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG23	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG22	30	0.14
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG23	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG22	30	0.14
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG23	30	0.14
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG22	30	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG23	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG22	30	0.14
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG23	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG11	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG12	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG13	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG21	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG22	30	0.14
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG23	30	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	26	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	26	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	26	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	26	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	26	0.14
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	26	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	11	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	28	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	28	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	28	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	28	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	28	0.14
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	28	0.14
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	21	0.14
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	21	0.14
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	21	0.14
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	21	0.14
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	21	0.14
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	21	0.14
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD11	40	0.14
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD12	40	0.14
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD13	40	0.14
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD21	40	0.14
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD22	40	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2410)	1:28:A:LEU:HG	1:69:A:LEU:HD23	40	0.14
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	2	0.14
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	2	0.14
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	2	0.14
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	2	0.14
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	2	0.14
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	2	0.14
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	34	0.14
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	34	0.14
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	34	0.14
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	34	0.14
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	34	0.14
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	34	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	17	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	17	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	17	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	17	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	17	0.14
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	17	0.14
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	4	0.14
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	4	0.14
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	14	0.14
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	14	0.14
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	14	0.14
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	14	0.14
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	14	0.14
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	14	0.14
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	14	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	6	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	6	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	6	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	22	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	22	0.14
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	22	0.14
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	36	0.14
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	36	0.14
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	36	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	17	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	17	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	17	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	23	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	23	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	23	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	35	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	35	0.14
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	35	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	5	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	5	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	5	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	22	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	22	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	22	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	23	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	23	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	23	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	37	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	37	0.14
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	37	0.14
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD11	7	0.14
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD12	7	0.14
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD13	7	0.14
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD2	39	0.14
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD3	39	0.14
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	18	0.14
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	18	0.14
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	18	0.14
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	20	0.14
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	20	0.14
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	20	0.14
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	25	0.14
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	25	0.14
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	25	0.14
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	12	0.14
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	12	0.14
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	12	0.14
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	12	0.14
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	23	0.14
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	23	0.14
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	23	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	23	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	30	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	30	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	30	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	38	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	38	0.14
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	38	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	19	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	19	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	19	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	23	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	23	0.14
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	23	0.14
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	35	0.14
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	35	0.14
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	33	0.14
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	36	0.14
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	2	0.14
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	2	0.14
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	2	0.14
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	18	0.14
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	25	0.14
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	29	0.14
(1,1104)	1:68:A:SER:HB2	1:69:A:LEU:HG	30	0.14
(1,1104)	1:68:A:SER:HB3	1:69:A:LEU:HG	30	0.14
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	18	0.14
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	18	0.14
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	18	0.14
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG21	19	0.14
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG22	19	0.14
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG23	19	0.14
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG21	19	0.14
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG22	19	0.14
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG23	19	0.14
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG21	29	0.14
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG22	29	0.14
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG23	29	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	29	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	29	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	29	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	34	0.14
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	34	0.14
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	11	0.14
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	11	0.14
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	11	0.14
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	16	0.14
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	16	0.14
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	16	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	7	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	7	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	7	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	14	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	14	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	14	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	20	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	20	0.14
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	20	0.14
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	33	0.14
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	33	0.14
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	33	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	18	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	18	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	18	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	20	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	20	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	20	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	21	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	21	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	21	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	31	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	31	0.14
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	31	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	14	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	14	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	14	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	18	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	18	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	18	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	32	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	32	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	32	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	36	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	36	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	36	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	40	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	40	0.14
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	40	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	21	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	21	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	21	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	33	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	33	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	33	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	34	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	34	0.14
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	34	0.14
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	32	0.14
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	32	0.14
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	32	0.14
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	36	0.14
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	36	0.14
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	36	0.14
(1,640)	1:37:A:THR:HG1	1:40:A:LEU:HD21	29	0.14
(1,640)	1:37:A:THR:HG1	1:40:A:LEU:HD22	29	0.14
(1,640)	1:37:A:THR:HG1	1:40:A:LEU:HD23	29	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	4	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	4	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	4	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	4	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	4	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	4	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	22	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	22	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	22	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	22	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	22	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	22	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	36	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	36	0.14
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	36	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	36	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	36	0.14
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	36	0.14
(1,439)	1:25:A:LEU:HD11	1:62:A:VAL:H	17	0.14
(1,439)	1:25:A:LEU:HD12	1:62:A:VAL:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:25:A:LEU:HD13	1:62:A:VAL:H	17	0.14
(1,439)	1:25:A:LEU:HD11	1:62:A:VAL:H	20	0.14
(1,439)	1:25:A:LEU:HD12	1:62:A:VAL:H	20	0.14
(1,439)	1:25:A:LEU:HD13	1:62:A:VAL:H	20	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	7	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	7	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	7	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	12	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	12	0.14
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	12	0.14
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	24	0.14
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	24	0.14
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	24	0.14
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	30	0.14
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	30	0.14
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	30	0.14
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	28	0.14
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	28	0.14
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	28	0.14
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	32	0.14
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	32	0.14
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	32	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	14	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	14	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	14	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	14	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	14	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	14	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	14	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	14	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	14	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	40	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	40	0.14
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	40	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	40	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	40	0.14
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	40	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	40	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	40	0.14
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	40	0.14
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	14	0.14
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	14	0.14
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	21	0.14
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	21	0.14
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	21	0.14
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	25	0.14
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	25	0.14
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	25	0.14
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	32	0.14
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	32	0.14
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	32	0.14
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	12	0.14
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	12	0.14
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	12	0.14
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	14	0.14
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	14	0.14
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	14	0.14
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	21	0.13
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	21	0.13
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	21	0.13
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	21	0.13
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	27	0.13
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	33	0.13
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	33	0.13
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	33	0.13
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	33	0.13
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	33	0.13
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	33	0.13
(1,2844)	1:77:A:LEU:HD11	1:103:A:LEU:H	31	0.13
(1,2844)	1:77:A:LEU:HD12	1:103:A:LEU:H	31	0.13
(1,2844)	1:77:A:LEU:HD13	1:103:A:LEU:H	31	0.13
(1,2844)	1:77:A:LEU:HD21	1:103:A:LEU:H	31	0.13
(1,2844)	1:77:A:LEU:HD22	1:103:A:LEU:H	31	0.13
(1,2844)	1:77:A:LEU:HD23	1:103:A:LEU:H	31	0.13
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	34	0.13
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	34	0.13
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	34	0.13
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	34	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	34	0.13
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	34	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG11	3	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG12	3	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG13	3	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG21	3	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG22	3	0.13
(1,2728)	1:60:A:GLU:HA	1:62:A:VAL:HG23	3	0.13
(1,2725)	1:59:A:ASP:HB2	1:62:A:VAL:HB	14	0.13
(1,2725)	1:59:A:ASP:HB3	1:62:A:VAL:HB	14	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG11	30	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG12	30	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG13	30	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG21	30	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG22	30	0.13
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG23	30	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	14	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	27	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	33	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	34	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	40	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	40	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	40	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	40	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	40	0.13
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	40	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	25	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	34	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	34	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	34	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	34	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	34	0.13
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	34	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	35	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	35	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	35	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	35	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	35	0.13
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	35	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	4	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	4	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	4	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	4	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	4	0.13
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	4	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	30	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	34	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	34	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	34	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	34	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	34	0.13
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	34	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	5	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	5	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	5	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	5	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	5	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	37	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	37	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	37	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	37	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	37	0.13
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	37	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	2	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	4	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	25	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	25	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	25	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	25	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	25	0.13
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	25	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	1	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	1	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	10	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	10	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	21	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	21	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	21	0.13
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	21	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG11	13	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG12	13	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG13	13	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG21	13	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG22	13	0.13
(1,2468)	1:31:A:LEU:HG	1:50:A:VAL:HG23	13	0.13
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	20	0.13
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	20	0.13
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	20	0.13
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	20	0.13
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	20	0.13
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	20	0.13
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	4	0.13
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	18	0.13
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	38	0.13
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	38	0.13
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	38	0.13
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	38	0.13
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	38	0.13
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	38	0.13
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	15	0.13
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	15	0.13
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	15	0.13
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	15	0.13
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	15	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	29	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	29	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	29	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	29	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	29	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	29	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	30	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	30	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	30	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	30	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	30	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	30	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	40	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	40	0.13
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	40	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	40	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	40	0.13
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	40	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	26	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	26	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	38	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	38	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	38	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	38	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	38	0.13
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	38	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	38	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	38	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	38	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	38	0.13
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	38	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	21	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	33	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	33	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	33	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	33	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	33	0.13
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	33	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	13	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	13	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	16	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	16	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	39	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	39	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	39	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	39	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	39	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	39	0.13
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	39	0.13
(1,2094)	1:16:A:VAL:HA	1:56:A:GLN:HE21	12	0.13
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	3	0.13
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	3	0.13
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	3	0.13
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	30	0.13
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	30	0.13
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	30	0.13
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	33	0.13
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	33	0.13
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	33	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	4	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	4	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	4	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	16	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	16	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	16	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	20	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	20	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	20	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	35	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	35	0.13
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	35	0.13
(1,1617)	1:14:A:LYS:HB2	1:15:A:MET:H	11	0.13
(1,1617)	1:14:A:LYS:HB3	1:15:A:MET:H	11	0.13
(1,1617)	1:14:A:LYS:HB2	1:15:A:MET:H	31	0.13
(1,1617)	1:14:A:LYS:HB3	1:15:A:MET:H	31	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	32	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	32	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	32	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	38	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	38	0.13
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	27	0.13
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	27	0.13
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	27	0.13
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	31	0.13
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	31	0.13
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	31	0.13
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	32	0.13
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	32	0.13
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	32	0.13
(1,1453)	1:101:A:LYS:HG2	1:102:A:ASP:HB3	39	0.13
(1,1453)	1:101:A:LYS:HG3	1:102:A:ASP:HB3	39	0.13
(1,1440)	1:38:A:LEU:HD11	1:42:A:GLN:HE21	26	0.13
(1,1440)	1:38:A:LEU:HD12	1:42:A:GLN:HE21	26	0.13
(1,1440)	1:38:A:LEU:HD13	1:42:A:GLN:HE21	26	0.13
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	8	0.13
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	8	0.13
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	8	0.13
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	8	0.13
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	18	0.13
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	18	0.13
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	18	0.13
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	18	0.13
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	23	0.13
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	23	0.13
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	23	0.13
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD11	39	0.13
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD12	39	0.13
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD13	39	0.13
(1,1307)	1:77:A:LEU:HD21	1:100:A:GLU:HA	14	0.13
(1,1307)	1:77:A:LEU:HD22	1:100:A:GLU:HA	14	0.13
(1,1307)	1:77:A:LEU:HD23	1:100:A:GLU:HA	14	0.13
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	29	0.13
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	29	0.13
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	29	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	4	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	4	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	4	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	12	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	12	0.13
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	12	0.13
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	21	0.13
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	22	0.13
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	22	0.13
(1,1166)	1:70:A:ILE:HD11	1:73:A:TRP:HH2	7	0.13
(1,1166)	1:70:A:ILE:HD12	1:73:A:TRP:HH2	7	0.13
(1,1166)	1:70:A:ILE:HD13	1:73:A:TRP:HH2	7	0.13
(1,1119)	1:69:A:LEU:HD11	1:73:A:TRP:HE3	29	0.13
(1,1119)	1:69:A:LEU:HD12	1:73:A:TRP:HE3	29	0.13
(1,1119)	1:69:A:LEU:HD13	1:73:A:TRP:HE3	29	0.13
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	36	0.13
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	39	0.13
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB1	29	0.13
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB2	29	0.13
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB3	29	0.13
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	19	0.13
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	19	0.13
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	19	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	30	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	30	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	30	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	31	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	31	0.13
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	31	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	25	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	25	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	25	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	36	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	36	0.13
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	36	0.13
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	8	0.13
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	8	0.13
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	8	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	12	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	12	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	12	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	32	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	32	0.13
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	32	0.13
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	31	0.13
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	31	0.13
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	31	0.13
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	14	0.13
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	14	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	4	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	4	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	4	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	39	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	39	0.13
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	39	0.13
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	14	0.13
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	14	0.13
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	14	0.13
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	17	0.13
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	17	0.13
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	17	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	3	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	3	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	3	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	10	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	10	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	10	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD21	13	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD22	13	0.13
(1,592)	1:74:A:LYS:H	1:76:A:LEU:HD23	13	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	12	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	12	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	12	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	12	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	12	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	12	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	32	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	32	0.13
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	32	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	32	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	32	0.13
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	32	0.13
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	30	0.13
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	30	0.13
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	30	0.13
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	30	0.13
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	30	0.13
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	30	0.13
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	30	0.13
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	30	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	30	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD11	36	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD12	36	0.13
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD13	36	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD11	36	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD12	36	0.13
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD13	36	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	6	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	6	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	6	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	19	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	19	0.13
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	19	0.13
(1,343)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	20	0.13
(1,343)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	20	0.13
(1,343)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	20	0.13
(1,343)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	20	0.13
(1,343)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	20	0.13
(1,343)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	20	0.13
(1,343)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	20	0.13
(1,343)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	20	0.13
(1,343)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	20	0.13
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	29	0.13
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	29	0.13
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	29	0.13
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	40	0.13
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	40	0.13
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	40	0.13
(1,324)	1:24:A:ALA:HB1	1:62:A:VAL:HB	6	0.13
(1,324)	1:24:A:ALA:HB2	1:62:A:VAL:HB	6	0.13
(1,324)	1:24:A:ALA:HB3	1:62:A:VAL:HB	6	0.13
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	25	0.13
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	25	0.13
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	25	0.13
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB1	18	0.13
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB2	18	0.13
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB3	18	0.13
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB1	18	0.13
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB2	18	0.13
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB3	18	0.13
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB1	18	0.13
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB3	18	0.13
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	39	0.13
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	39	0.13
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	39	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	4	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	4	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	4	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	4	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	4	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	4	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	4	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	4	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	4	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	21	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	21	0.13
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	21	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	21	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	21	0.13
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	21	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	21	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	21	0.13
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	21	0.13
(1,129)	1:9:A:ALA:HB1	1:13:A:ASP:HB3	16	0.13
(1,129)	1:9:A:ALA:HB2	1:13:A:ASP:HB3	16	0.13
(1,129)	1:9:A:ALA:HB3	1:13:A:ASP:HB3	16	0.13
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG11	29	0.13
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG12	29	0.13
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG13	29	0.13
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	29	0.13
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	29	0.13
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	29	0.13
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	15	0.13
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	15	0.13
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	15	0.13
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	16	0.13
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	16	0.13
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	16	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD11	4	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD12	4	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD13	4	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD11	4	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD13	4	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD11	4	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD12	4	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD13	4	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD11	40	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD12	40	0.13
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD13	40	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD11	40	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD12	40	0.13
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD13	40	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD11	40	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD12	40	0.13
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD13	40	0.13
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	31	0.12
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	31	0.12
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	31	0.12
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	31	0.12
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	31	0.12
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	31	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	2	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	20	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	23	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	23	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	23	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	23	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	23	0.12
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	23	0.12
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB2	38	0.12
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB3	38	0.12
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB2	38	0.12
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB3	38	0.12
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	25	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	25	0.12
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	25	0.12
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	25	0.12
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	25	0.12
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	25	0.12
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	26	0.12
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	26	0.12
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	26	0.12
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	26	0.12
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	26	0.12
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	26	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD11	20	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD12	20	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD13	20	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD21	20	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD22	20	0.12
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD23	20	0.12
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB2	4	0.12
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB3	4	0.12
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB2	4	0.12
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB3	4	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	18	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	20	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	21	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	29	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	29	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	29	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	29	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	29	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	29	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	32	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	32	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	32	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	32	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	32	0.12
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	32	0.12
(1,2619)	1:45:A:ARG:HG2	1:48:A:MET:H	25	0.12
(1,2619)	1:45:A:ARG:HG3	1:48:A:MET:H	25	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	5	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	11	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	23	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	27	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	28	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	28	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	28	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	28	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	28	0.12
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	28	0.12
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	21	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	21	0.12
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	21	0.12
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	21	0.12
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	21	0.12
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	21	0.12
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	27	0.12
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	31	0.12
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	31	0.12
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	31	0.12
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	31	0.12
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	31	0.12
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	31	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	24	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	26	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	37	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	37	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	37	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	37	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	37	0.12
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	37	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	12	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	12	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	12	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	12	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	12	0.12
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	12	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	14	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	14	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	14	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	14	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	14	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	20	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	33	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	33	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	33	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	33	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	33	0.12
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	33	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	2	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	6	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	28	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	28	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	28	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	28	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	28	0.12
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	12	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	24	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	24	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	24	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	24	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	24	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	24	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	28	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	30	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	30	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	30	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	30	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	30	0.12
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	30	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD11	4	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD12	4	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD13	4	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD21	4	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD22	4	0.12
(1,2502)	1:36:A:MET:HA	1:40:A:LEU:HD23	4	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD11	40	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD12	40	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD13	40	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD21	40	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD22	40	0.12
(1,2500)	1:36:A:MET:H	1:40:A:LEU:HD23	40	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	29	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	29	0.12
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	29	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	29	0.12
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	29	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG11	40	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD11	1:50:A:VAL:HG23	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG11	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD12	1:50:A:VAL:HG23	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG11	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD13	1:50:A:VAL:HG23	40	0.12
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG11	40	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD21	1:50:A:VAL:HG23	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG11	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD22	1:50:A:VAL:HG23	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG11	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG12	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG13	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG21	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG22	40	0.12
(1,2477)	1:31:A:LEU:HD23	1:50:A:VAL:HG23	40	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	17	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD11	35	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD12	35	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD13	35	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD21	35	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD22	35	0.12
(1,2469)	1:31:A:LEU:HG	1:69:A:LEU:HD23	35	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	2	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	33	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	37	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	37	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	37	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	37	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	37	0.12
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	37	0.12
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	10	0.12
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	10	0.12
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	10	0.12
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	10	0.12
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	10	0.12
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	10	0.12
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	23	0.12
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	40	0.12
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	40	0.12
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	40	0.12
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	40	0.12
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	40	0.12
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	40	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD11	6	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD12	6	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD13	6	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD21	6	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD22	6	0.12
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD23	6	0.12
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB2	40	0.12
(1,2373)	1:26:A:ASP:HB2	1:27:A:LEU:HB3	40	0.12
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	7	0.12
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	30	0.12
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	30	0.12
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	30	0.12
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	30	0.12
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	30	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	30	0.12
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	16	0.12
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	26	0.12
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	35	0.12
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	35	0.12
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	35	0.12
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	35	0.12
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	35	0.12
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	35	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	7	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	7	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	7	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	7	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	7	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	7	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	19	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	19	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	19	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	19	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	19	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	19	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	26	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	26	0.12
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	26	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	26	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	26	0.12
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	26	0.12
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB1	20	0.12
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB2	20	0.12
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB3	20	0.12
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB1	20	0.12
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB3	20	0.12
(1,2239)	1:13:A:ASP:HB2	1:52:A:ALA:HB1	39	0.12
(1,2239)	1:13:A:ASP:HB2	1:52:A:ALA:HB2	39	0.12
(1,2239)	1:13:A:ASP:HB2	1:52:A:ALA:HB3	39	0.12
(1,2239)	1:13:A:ASP:HB3	1:52:A:ALA:HB1	39	0.12
(1,2239)	1:13:A:ASP:HB3	1:52:A:ALA:HB2	39	0.12
(1,2239)	1:13:A:ASP:HB3	1:52:A:ALA:HB3	39	0.12
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	16	0.12
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	16	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	7	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	7	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	7	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	7	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	7	0.12
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	7	0.12
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	25	0.12
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	25	0.12
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	35	0.12
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	35	0.12
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	35	0.12
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	35	0.12
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	35	0.12
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	35	0.12
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	35	0.12
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	33	0.12
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	33	0.12
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	33	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	1	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	1	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	1	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	6	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	6	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	6	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	7	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	7	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	7	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	14	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	14	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	14	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	24	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	24	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	24	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	26	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	26	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	26	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	32	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	32	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	32	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	37	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	37	0.12
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	37	0.12
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	24	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	1	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	1	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	1	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	5	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	5	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	5	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG11	28	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG12	28	0.12
(1,1608)	1:14:A:LYS:H	1:16:A:VAL:HG13	28	0.12
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD11	17	0.12
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD12	17	0.12
(1,1587)	1:11:A:LYS:H	1:27:A:LEU:HD13	17	0.12
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	12	0.12
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	12	0.12
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	12	0.12
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	33	0.12
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	33	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	33	0.12
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	21	0.12
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	21	0.12
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	21	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	6	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	6	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	6	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	6	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	9	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	9	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	9	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	9	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	10	0.12
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	10	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	10	0.12
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	10	0.12
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	17	0.12
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	17	0.12
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	17	0.12
(1,1349)	1:41:A:LEU:H	1:103:A:LEU:HD11	29	0.12
(1,1349)	1:41:A:LEU:H	1:103:A:LEU:HD12	29	0.12
(1,1349)	1:41:A:LEU:H	1:103:A:LEU:HD13	29	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD11	31	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD12	31	0.12
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD13	31	0.12
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	18	0.12
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	18	0.12
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	18	0.12
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	17	0.12
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	17	0.12
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	17	0.12
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	4	0.12
(1,1131)	1:32:A:LYS:HE2	1:69:A:LEU:HD21	29	0.12
(1,1131)	1:32:A:LYS:HE2	1:69:A:LEU:HD22	29	0.12
(1,1131)	1:32:A:LYS:HE2	1:69:A:LEU:HD23	29	0.12
(1,1131)	1:32:A:LYS:HE3	1:69:A:LEU:HD21	29	0.12
(1,1131)	1:32:A:LYS:HE3	1:69:A:LEU:HD22	29	0.12
(1,1131)	1:32:A:LYS:HE3	1:69:A:LEU:HD23	29	0.12
(1,1119)	1:69:A:LEU:HD11	1:73:A:TRP:HE3	34	0.12
(1,1119)	1:69:A:LEU:HD12	1:73:A:TRP:HE3	34	0.12
(1,1119)	1:69:A:LEU:HD13	1:73:A:TRP:HE3	34	0.12
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	21	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	40	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB1	32	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB2	32	0.12
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB3	32	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	23	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	23	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	23	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	37	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	37	0.12
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	37	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	14	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	14	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	14	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	32	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	32	0.12
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	32	0.12
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	30	0.12
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	30	0.12
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	30	0.12
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	40	0.12
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	10	0.12
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	10	0.12
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	10	0.12
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	14	0.12
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	14	0.12
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	14	0.12
(1,924)	1:53:A:ILE:HG21	1:62:A:VAL:H	29	0.12
(1,924)	1:53:A:ILE:HG22	1:62:A:VAL:H	29	0.12
(1,924)	1:53:A:ILE:HG23	1:62:A:VAL:H	29	0.12
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	34	0.12
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	34	0.12
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	34	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	2	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	2	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	2	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	6	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	6	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	6	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	18	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	18	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	18	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	27	0.12
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	27	0.12
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	7	0.12
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	7	0.12
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	7	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	6	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	6	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	6	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	7	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	7	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	7	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	19	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	19	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	19	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	29	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	29	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	29	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	39	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	39	0.12
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	39	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	12	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	12	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	12	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	20	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	20	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	20	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	21	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	21	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	21	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	27	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	27	0.12
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	27	0.12
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD11	40	0.12
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD12	40	0.12
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD13	40	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	7	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	7	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	7	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	12	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	12	0.12
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	12	0.12
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	27	0.12
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	27	0.12
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	33	0.12
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	33	0.12
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	33	0.12
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	35	0.12
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	35	0.12
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	35	0.12
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	40	0.12
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	40	0.12
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	40	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	1	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	1	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	1	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	1	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	1	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	1	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	2	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	2	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	2	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	2	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	2	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	2	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	6	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	6	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	6	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	6	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	6	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	6	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	7	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	7	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	7	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	7	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	7	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	7	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	19	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	19	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	19	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	19	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	19	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	19	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	28	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	28	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	28	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	28	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	28	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	28	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	38	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	38	0.12
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	38	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	38	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	38	0.12
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	38	0.12
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	2	0.12
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	2	0.12
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	2	0.12
(1,324)	1:24:A:ALA:HB1	1:62:A:VAL:HB	34	0.12
(1,324)	1:24:A:ALA:HB2	1:62:A:VAL:HB	34	0.12
(1,324)	1:24:A:ALA:HB3	1:62:A:VAL:HB	34	0.12
(1,313)	1:24:A:ALA:HB1	1:53:A:ILE:H	18	0.12
(1,313)	1:24:A:ALA:HB2	1:53:A:ILE:H	18	0.12
(1,313)	1:24:A:ALA:HB3	1:53:A:ILE:H	18	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	21	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	21	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	21	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	36	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	36	0.12
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	36	0.12
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	8	0.12
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	8	0.12
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	8	0.12
(1,270)	1:16:A:VAL:HG21	1:56:A:GLN:HE21	24	0.12
(1,270)	1:16:A:VAL:HG22	1:56:A:GLN:HE21	24	0.12
(1,270)	1:16:A:VAL:HG23	1:56:A:GLN:HE21	24	0.12
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	7	0.12
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	7	0.12
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	7	0.12
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	30	0.12
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	30	0.12
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	30	0.12
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	6	0.12
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	6	0.12
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	6	0.12
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	19	0.12
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	19	0.12
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	34	0.12
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	34	0.12
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	34	0.12
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	37	0.12
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	37	0.12
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	37	0.12
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD11	39	0.12
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD12	39	0.12
(1,34)	1:1:A:MET:HE1	1:34:A:ILE:HD13	39	0.12
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD11	39	0.12
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD12	39	0.12
(1,34)	1:1:A:MET:HE2	1:34:A:ILE:HD13	39	0.12
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD11	39	0.12
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD12	39	0.12
(1,34)	1:1:A:MET:HE3	1:34:A:ILE:HD13	39	0.12
(1,2844)	1:77:A:LEU:HD11	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD12	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD13	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD21	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD22	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD23	1:103:A:LEU:H	29	0.11
(1,2844)	1:77:A:LEU:HD11	1:103:A:LEU:H	33	0.11
(1,2844)	1:77:A:LEU:HD12	1:103:A:LEU:H	33	0.11
(1,2844)	1:77:A:LEU:HD13	1:103:A:LEU:H	33	0.11
(1,2844)	1:77:A:LEU:HD21	1:103:A:LEU:H	33	0.11
(1,2844)	1:77:A:LEU:HD22	1:103:A:LEU:H	33	0.11
(1,2844)	1:77:A:LEU:HD23	1:103:A:LEU:H	33	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	17	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	18	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	31	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	31	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	31	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	31	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	31	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	31	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD11	34	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD12	34	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD13	34	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD21	34	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD22	34	0.11
(1,2835)	1:77:A:LEU:HG	1:103:A:LEU:HD23	34	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD11	39	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD12	39	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD13	39	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD21	39	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD22	39	0.11
(1,2802)	1:74:A:LYS:H	1:77:A:LEU:HD23	39	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	1	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	16	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	18	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	21	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	32	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	32	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	32	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	32	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	32	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	32	0.11
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	33	0.11
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	33	0.11
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	33	0.11
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	33	0.11
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	33	0.11
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	33	0.11
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB2	14	0.11
(1,2695)	1:54:A:ARG:HG2	1:57:A:SER:HB3	14	0.11
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB2	14	0.11
(1,2695)	1:54:A:ARG:HG3	1:57:A:SER:HB3	14	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG11	7	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG12	7	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG13	7	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG21	7	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG22	7	0.11
(1,2693)	1:54:A:ARG:HA	1:62:A:VAL:HG23	7	0.11
(1,2660)	1:50:A:VAL:HG11	1:67:A:LYS:H	32	0.11
(1,2660)	1:50:A:VAL:HG12	1:67:A:LYS:H	32	0.11
(1,2660)	1:50:A:VAL:HG13	1:67:A:LYS:H	32	0.11
(1,2660)	1:50:A:VAL:HG21	1:67:A:LYS:H	32	0.11
(1,2660)	1:50:A:VAL:HG22	1:67:A:LYS:H	32	0.11
(1,2660)	1:50:A:VAL:HG23	1:67:A:LYS:H	32	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	7	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	25	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	25	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	25	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	25	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	25	0.11
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	25	0.11
(1,2578)	1:41:A:LEU:HD11	1:42:A:GLN:H	30	0.11
(1,2578)	1:41:A:LEU:HD12	1:42:A:GLN:H	30	0.11
(1,2578)	1:41:A:LEU:HD13	1:42:A:GLN:H	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2578)	1:41:A:LEU:HD21	1:42:A:GLN:H	30	0.11
(1,2578)	1:41:A:LEU:HD22	1:42:A:GLN:H	30	0.11
(1,2578)	1:41:A:LEU:HD23	1:42:A:GLN:H	30	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	8	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	8	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	8	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	8	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	8	0.11
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	8	0.11
(1,2564)	1:40:A:LEU:HD11	1:45:A:ARG:H	25	0.11
(1,2564)	1:40:A:LEU:HD12	1:45:A:ARG:H	25	0.11
(1,2564)	1:40:A:LEU:HD13	1:45:A:ARG:H	25	0.11
(1,2564)	1:40:A:LEU:HD21	1:45:A:ARG:H	25	0.11
(1,2564)	1:40:A:LEU:HD22	1:45:A:ARG:H	25	0.11
(1,2564)	1:40:A:LEU:HD23	1:45:A:ARG:H	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	2	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	25	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	29	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	29	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	29	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	29	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	29	0.11
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	29	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	5	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	6	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	6	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	6	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	6	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	6	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	15	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD11	18	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD12	18	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD13	18	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD21	18	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD22	18	0.11
(1,2546)	1:39:A:GLU:HA	1:40:A:LEU:HD23	18	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	8	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	9	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	10	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	15	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	16	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	16	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	16	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	16	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	16	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	17	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	23	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	26	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	38	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	38	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	38	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	38	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	38	0.11
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	38	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	6	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	22	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	35	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	35	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	35	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	35	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	35	0.11
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	35	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	38	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	38	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	38	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	38	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	38	0.11
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	38	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	7	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	14	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	17	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	19	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	27	0.11
(1,2411)	1:28:A:LEU:HD11	1:29:A:LYS:H	31	0.11
(1,2411)	1:28:A:LEU:HD12	1:29:A:LYS:H	31	0.11
(1,2411)	1:28:A:LEU:HD13	1:29:A:LYS:H	31	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:28:A:LEU:HD21	1:29:A:LYS:H	31	0.11
(1,2411)	1:28:A:LEU:HD22	1:29:A:LYS:H	31	0.11
(1,2411)	1:28:A:LEU:HD23	1:29:A:LYS:H	31	0.11
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	22	0.11
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	22	0.11
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	22	0.11
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	22	0.11
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	22	0.11
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	22	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	11	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	11	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	11	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	11	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	11	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	11	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	20	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	20	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	20	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	20	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	20	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	20	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG21	22	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG22	22	0.11
(1,2269)	1:15:A:MET:HG2	1:53:A:ILE:HG23	22	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG21	22	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG22	22	0.11
(1,2269)	1:15:A:MET:HG3	1:53:A:ILE:HG23	22	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB1	21	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB2	21	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB3	21	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB1	21	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB2	21	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB3	21	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB1	25	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB2	25	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB3	25	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB1	25	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB2	25	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB3	25	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB1	40	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB2	40	0.11
(1,2267)	1:15:A:MET:HG2	1:21:A:ALA:HB3	40	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB1	40	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB2	40	0.11
(1,2267)	1:15:A:MET:HG3	1:21:A:ALA:HB3	40	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	13	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	13	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG11	22	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG12	22	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG13	22	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG21	22	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG22	22	0.11
(1,2265)	1:15:A:MET:HG2	1:16:A:VAL:HG23	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG11	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG12	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG13	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG21	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG22	22	0.11
(1,2265)	1:15:A:MET:HG3	1:16:A:VAL:HG23	22	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	6	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	25	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	25	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	25	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	25	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	25	0.11
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	25	0.11
(1,2237)	1:13:A:ASP:HB2	1:16:A:VAL:HB	6	0.11
(1,2237)	1:13:A:ASP:HB3	1:16:A:VAL:HB	6	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	13	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	13	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	13	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	13	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	13	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	31	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	31	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	31	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	31	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	31	0.11
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	31	0.11
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	8	0.11
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	8	0.11
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	8	0.11
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	8	0.11
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	8	0.11
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	8	0.11
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	8	0.11
(1,1990)	1:70:A:ILE:HD11	1:71:A:LYS:H	29	0.11
(1,1990)	1:70:A:ILE:HD12	1:71:A:LYS:H	29	0.11
(1,1990)	1:70:A:ILE:HD13	1:71:A:LYS:H	29	0.11
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	31	0.11
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	31	0.11
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	31	0.11
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	34	0.11
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	34	0.11
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	34	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	12	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	12	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	12	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	23	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	23	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	23	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD21	33	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD22	33	0.11
(1,1765)	1:39:A:GLU:H	1:76:A:LEU:HD23	33	0.11
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	35	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	7	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	7	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	7	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	26	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	26	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	26	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	36	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	36	0.11
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	36	0.11
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD11	33	0.11
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD12	33	0.11
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD13	33	0.11
(1,1496)	1:70:A:ILE:HG21	1:73:A:TRP:HB3	40	0.11
(1,1496)	1:70:A:ILE:HG22	1:73:A:TRP:HB3	40	0.11
(1,1496)	1:70:A:ILE:HG23	1:73:A:TRP:HB3	40	0.11
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	14	0.11
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	14	0.11
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	14	0.11
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	30	0.11
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	30	0.11
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	30	0.11
(1,1473)	1:1:A:MET:HE1	1:36:A:MET:H	33	0.11
(1,1473)	1:1:A:MET:HE2	1:36:A:MET:H	33	0.11
(1,1473)	1:1:A:MET:HE3	1:36:A:MET:H	33	0.11
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	2	0.11
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	2	0.11
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	2	0.11
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	2	0.11
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE2	11	0.11
(1,1436)	1:72:A:SER:HB2	1:75:A:LYS:HE3	11	0.11
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE2	11	0.11
(1,1436)	1:72:A:SER:HB3	1:75:A:LYS:HE3	11	0.11
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	28	0.11
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	28	0.11
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	28	0.11
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	28	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	19	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	19	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	19	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD21	23	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD22	23	0.11
(1,1364)	1:100:A:GLU:H	1:103:A:LEU:HD23	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD21	40	0.11
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD22	40	0.11
(1,1361)	1:42:A:GLN:HE21	1:103:A:LEU:HD23	40	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD11	21	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD12	21	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD13	21	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD11	30	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD12	30	0.11
(1,1330)	1:102:A:ASP:HB2	1:103:A:LEU:HD13	30	0.11
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	39	0.11
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	39	0.11
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	39	0.11
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	40	0.11
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	40	0.11
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	40	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	2	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	2	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	2	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	15	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	15	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	15	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	16	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	16	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	16	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB1	37	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB2	37	0.11
(1,1271)	1:28:A:LEU:HG	1:66:A:ALA:HB3	37	0.11
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD2	15	0.11
(1,1268)	1:75:A:LYS:HA	1:75:A:LYS:HD3	15	0.11
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	6	0.11
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	7	0.11
(1,1135)	1:69:A:LEU:HD21	1:73:A:TRP:HE3	29	0.11
(1,1135)	1:69:A:LEU:HD22	1:73:A:TRP:HE3	29	0.11
(1,1135)	1:69:A:LEU:HD23	1:73:A:TRP:HE3	29	0.11
(1,1133)	1:68:A:SER:HB2	1:69:A:LEU:HD21	32	0.11
(1,1133)	1:68:A:SER:HB2	1:69:A:LEU:HD22	32	0.11
(1,1133)	1:68:A:SER:HB2	1:69:A:LEU:HD23	32	0.11
(1,1133)	1:68:A:SER:HB3	1:69:A:LEU:HD21	32	0.11
(1,1133)	1:68:A:SER:HB3	1:69:A:LEU:HD22	32	0.11
(1,1133)	1:68:A:SER:HB3	1:69:A:LEU:HD23	32	0.11
(1,1119)	1:69:A:LEU:HD11	1:73:A:TRP:HE3	21	0.11
(1,1119)	1:69:A:LEU:HD12	1:73:A:TRP:HE3	21	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:69:A:LEU:HD13	1:73:A:TRP:HE3	21	0.11
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	14	0.11
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	20	0.11
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	33	0.11
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB1	34	0.11
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB2	34	0.11
(1,1069)	1:28:A:LEU:HB2	1:66:A:ALA:HB3	34	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	2	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	2	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	2	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	15	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	15	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	15	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	22	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	22	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	22	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	26	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	26	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	26	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD21	35	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD22	35	0.11
(1,1038)	1:29:A:LYS:H	1:65:A:LEU:HD23	35	0.11
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG21	16	0.11
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG22	16	0.11
(1,1011)	1:54:A:ARG:HG2	1:63:A:THR:HG23	16	0.11
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG21	16	0.11
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG22	16	0.11
(1,1011)	1:54:A:ARG:HG3	1:63:A:THR:HG23	16	0.11
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG21	14	0.11
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG22	14	0.11
(1,995)	1:25:A:LEU:H	1:62:A:VAL:HG23	14	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	33	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	33	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	33	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	36	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	36	0.11
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	36	0.11
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	32	0.11
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	32	0.11
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	32	0.11
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	25	0.11
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	29	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	31	0.11
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	34	0.11
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	36	0.11
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	36	0.11
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	36	0.11
(1,862)	1:52:A:ALA:HB1	1:55:A:LYS:HE2	25	0.11
(1,862)	1:52:A:ALA:HB1	1:55:A:LYS:HE3	25	0.11
(1,862)	1:52:A:ALA:HB2	1:55:A:LYS:HE2	25	0.11
(1,862)	1:52:A:ALA:HB2	1:55:A:LYS:HE3	25	0.11
(1,862)	1:52:A:ALA:HB3	1:55:A:LYS:HE2	25	0.11
(1,862)	1:52:A:ALA:HB3	1:55:A:LYS:HE3	25	0.11
(1,820)	1:46:A:ILE:HG21	1:50:A:VAL:HG11	34	0.11
(1,820)	1:46:A:ILE:HG21	1:50:A:VAL:HG12	34	0.11
(1,820)	1:46:A:ILE:HG21	1:50:A:VAL:HG13	34	0.11
(1,820)	1:46:A:ILE:HG22	1:50:A:VAL:HG11	34	0.11
(1,820)	1:46:A:ILE:HG22	1:50:A:VAL:HG12	34	0.11
(1,820)	1:46:A:ILE:HG22	1:50:A:VAL:HG13	34	0.11
(1,820)	1:46:A:ILE:HG23	1:50:A:VAL:HG11	34	0.11
(1,820)	1:46:A:ILE:HG23	1:50:A:VAL:HG12	34	0.11
(1,820)	1:46:A:ILE:HG23	1:50:A:VAL:HG13	34	0.11
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG21	22	0.11
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG22	22	0.11
(1,794)	1:42:A:GLN:H	1:46:A:ILE:HG23	22	0.11
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	4	0.11
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	4	0.11
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	4	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	4	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	4	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	4	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	12	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	12	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	12	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	17	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	17	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	17	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	27	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	27	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	27	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD11	35	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD12	35	0.11
(1,769)	1:12:A:MET:H	1:46:A:ILE:HD13	35	0.11
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	6	0.11
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	6	0.11
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD11	7	0.11
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD12	7	0.11
(1,763)	1:44:A:THR:HG1	1:46:A:ILE:HD13	7	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	20	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	20	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	20	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	27	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	27	0.11
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	27	0.11
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	4	0.11
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	4	0.11
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	4	0.11
(1,643)	1:5:A:VAL:H	1:40:A:LEU:HD21	2	0.11
(1,643)	1:5:A:VAL:H	1:40:A:LEU:HD22	2	0.11
(1,643)	1:5:A:VAL:H	1:40:A:LEU:HD23	2	0.11
(1,625)	1:37:A:THR:HG1	1:40:A:LEU:HD11	40	0.11
(1,625)	1:37:A:THR:HG1	1:40:A:LEU:HD12	40	0.11
(1,625)	1:37:A:THR:HG1	1:40:A:LEU:HD13	40	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	15	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	15	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	15	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	15	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	15	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	15	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	31	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	31	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	31	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	31	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	31	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	31	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	37	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	37	0.11
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	37	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	37	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	37	0.11
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	37	0.11
(1,461)	1:32:A:LYS:HG2	1:34:A:ILE:H	21	0.11
(1,461)	1:32:A:LYS:HG3	1:34:A:ILE:H	21	0.11
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	18	0.11
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	18	0.11
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	18	0.11
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	18	0.11
(1,458)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	18	0.11
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	18	0.11
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	18	0.11
(1,458)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	18	0.11
(1,439)	1:25:A:LEU:HD11	1:62:A:VAL:H	6	0.11
(1,439)	1:25:A:LEU:HD12	1:62:A:VAL:H	6	0.11
(1,439)	1:25:A:LEU:HD13	1:62:A:VAL:H	6	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	23	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	23	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	23	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	30	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	30	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	30	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	37	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	37	0.11
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	37	0.11
(1,340)	1:25:A:LEU:HD11	1:26:A:ASP:H	5	0.11
(1,340)	1:25:A:LEU:HD12	1:26:A:ASP:H	5	0.11
(1,340)	1:25:A:LEU:HD13	1:26:A:ASP:H	5	0.11
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	39	0.11
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	39	0.11
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	39	0.11
(1,195)	1:15:A:MET:HE1	1:26:A:ASP:HB3	17	0.11
(1,195)	1:15:A:MET:HE2	1:26:A:ASP:HB3	17	0.11
(1,195)	1:15:A:MET:HE3	1:26:A:ASP:HB3	17	0.11
(1,179)	1:12:A:MET:HE1	1:50:A:VAL:H	34	0.11
(1,179)	1:12:A:MET:HE2	1:50:A:VAL:H	34	0.11
(1,179)	1:12:A:MET:HE3	1:50:A:VAL:H	34	0.11
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE1	10	0.11
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE2	10	0.11
(1,131)	1:9:A:ALA:HB1	1:12:A:MET:HE3	10	0.11
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE1	10	0.11
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE2	10	0.11
(1,131)	1:9:A:ALA:HB2	1:12:A:MET:HE3	10	0.11
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE1	10	0.11
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE2	10	0.11
(1,131)	1:9:A:ALA:HB3	1:12:A:MET:HE3	10	0.11
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG11	6	0.11
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG12	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:3:A:ASP:HB3	1:6:A:VAL:HG13	6	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	6	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	6	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	6	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	19	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	19	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	19	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	27	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	27	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	27	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	33	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	33	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	33	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	35	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	35	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	35	0.11
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	39	0.11
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	39	0.11
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	39	0.11
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	14	0.11
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	14	0.11
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	14	0.11
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	21	0.11
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	21	0.11
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	21	0.11
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	31	0.11
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	31	0.11
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	31	0.11
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	5	0.11
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	5	0.11
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	5	0.11
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	13	0.11
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	13	0.11
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	13	0.11
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	17	0.11
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	17	0.11
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	17	0.11
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	22	0.11
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	22	0.11
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	22	0.11
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	24	0.11
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	24	0.11
(1,44)	1:1:A:MET:HA	1:4:A:GLU:HG2	40	0.11
(1,44)	1:1:A:MET:HA	1:4:A:GLU:HG3	40	0.11
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	14	0.1
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	14	0.1
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	14	0.1
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	14	0.1
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB2	30	0.1
(1,2862)	1:98:A:ASN:HB2	1:101:A:LYS:HB3	30	0.1
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB2	30	0.1
(1,2862)	1:98:A:ASN:HB3	1:101:A:LYS:HB3	30	0.1
(1,2848)	1:77:A:LEU:HD11	1:104:A:PHE:H	20	0.1
(1,2848)	1:77:A:LEU:HD12	1:104:A:PHE:H	20	0.1
(1,2848)	1:77:A:LEU:HD13	1:104:A:PHE:H	20	0.1
(1,2848)	1:77:A:LEU:HD21	1:104:A:PHE:H	20	0.1
(1,2848)	1:77:A:LEU:HD22	1:104:A:PHE:H	20	0.1
(1,2848)	1:77:A:LEU:HD23	1:104:A:PHE:H	20	0.1
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB2	14	0.1
(1,2833)	1:77:A:LEU:HB2	1:78:A:ASP:HB3	14	0.1
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB2	14	0.1
(1,2833)	1:77:A:LEU:HB3	1:78:A:ASP:HB3	14	0.1
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	2	0.1
(1,2749)	1:62:A:VAL:HG11	1:67:A:LYS:H	36	0.1
(1,2749)	1:62:A:VAL:HG12	1:67:A:LYS:H	36	0.1
(1,2749)	1:62:A:VAL:HG13	1:67:A:LYS:H	36	0.1
(1,2749)	1:62:A:VAL:HG21	1:67:A:LYS:H	36	0.1
(1,2749)	1:62:A:VAL:HG22	1:67:A:LYS:H	36	0.1
(1,2749)	1:62:A:VAL:HG23	1:67:A:LYS:H	36	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD11	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD12	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD13	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD21	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD22	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD23	25	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD11	31	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD12	31	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD13	31	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD21	31	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD22	31	0.1
(1,2740)	1:62:A:VAL:HA	1:65:A:LEU:HD23	31	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG11	36	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG12	36	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG13	36	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG21	36	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG22	36	0.1
(1,2623)	1:46:A:ILE:HB	1:50:A:VAL:HG23	36	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	1	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD11	16	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD12	16	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD13	16	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD21	16	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD22	16	0.1
(1,2577)	1:41:A:LEU:HG	1:77:A:LEU:HD23	16	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	22	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD11	38	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD12	38	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD13	38	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD21	38	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD22	38	0.1
(1,2557)	1:40:A:LEU:HB3	1:41:A:LEU:HD23	38	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD11	36	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD12	36	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD13	36	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD21	36	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD22	36	0.1
(1,2555)	1:40:A:LEU:HB2	1:41:A:LEU:HD23	36	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	11	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	11	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	11	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	11	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	11	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD11	35	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD12	35	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD13	35	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD21	35	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD22	35	0.1
(1,2544)	1:39:A:GLU:H	1:41:A:LEU:HD23	35	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	5	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	11	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	17	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD11	38	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD12	38	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD13	38	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD21	38	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD22	38	0.1
(1,2514)	1:37:A:THR:H	1:41:A:LEU:HD23	38	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD13	8	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD11	1:69:A:LEU:HD23	8	0.1
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD13	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD12	1:69:A:LEU:HD23	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD13	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD13	1:69:A:LEU:HD23	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD13	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD21	1:69:A:LEU:HD23	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD13	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD22	1:69:A:LEU:HD23	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD11	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD12	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD13	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD21	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD22	8	0.1
(1,2479)	1:31:A:LEU:HD23	1:69:A:LEU:HD23	8	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD11	19	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD12	19	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD13	19	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD21	19	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD22	19	0.1
(1,2458)	1:30:A:GLU:HG3	1:31:A:LEU:HD23	19	0.1
(1,2433)	1:28:A:LEU:HD11	1:69:A:LEU:HB3	3	0.1
(1,2433)	1:28:A:LEU:HD12	1:69:A:LEU:HB3	3	0.1
(1,2433)	1:28:A:LEU:HD13	1:69:A:LEU:HB3	3	0.1
(1,2433)	1:28:A:LEU:HD21	1:69:A:LEU:HB3	3	0.1
(1,2433)	1:28:A:LEU:HD22	1:69:A:LEU:HB3	3	0.1
(1,2433)	1:28:A:LEU:HD23	1:69:A:LEU:HB3	3	0.1
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD11	21	0.1
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD12	21	0.1
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD13	21	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD21	21	0.1
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD22	21	0.1
(1,2379)	1:27:A:LEU:H	1:28:A:LEU:HD23	21	0.1
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	29	0.1
(1,2355)	1:25:A:LEU:HD11	1:29:A:LYS:H	40	0.1
(1,2355)	1:25:A:LEU:HD12	1:29:A:LYS:H	40	0.1
(1,2355)	1:25:A:LEU:HD13	1:29:A:LYS:H	40	0.1
(1,2355)	1:25:A:LEU:HD21	1:29:A:LYS:H	40	0.1
(1,2355)	1:25:A:LEU:HD22	1:29:A:LYS:H	40	0.1
(1,2355)	1:25:A:LEU:HD23	1:29:A:LYS:H	40	0.1
(1,2354)	1:25:A:LEU:HD11	1:26:A:ASP:HB2	28	0.1
(1,2354)	1:25:A:LEU:HD12	1:26:A:ASP:HB2	28	0.1
(1,2354)	1:25:A:LEU:HD13	1:26:A:ASP:HB2	28	0.1
(1,2354)	1:25:A:LEU:HD21	1:26:A:ASP:HB2	28	0.1
(1,2354)	1:25:A:LEU:HD22	1:26:A:ASP:HB2	28	0.1
(1,2354)	1:25:A:LEU:HD23	1:26:A:ASP:HB2	28	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD11	34	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD12	34	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD13	34	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD21	34	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD22	34	0.1
(1,2243)	1:14:A:LYS:H	1:27:A:LEU:HD23	34	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	5	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD11	26	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD12	26	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD13	26	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD21	26	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD22	26	0.1
(1,2188)	1:10:A:LYS:H	1:27:A:LEU:HD23	26	0.1
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD2	19	0.1
(1,2144)	1:6:A:VAL:HG11	1:7:A:ARG:HD3	19	0.1
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD2	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2144)	1:6:A:VAL:HG12	1:7:A:ARG:HD3	19	0.1
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD2	19	0.1
(1,2144)	1:6:A:VAL:HG13	1:7:A:ARG:HD3	19	0.1
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD2	19	0.1
(1,2144)	1:6:A:VAL:HG21	1:7:A:ARG:HD3	19	0.1
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD2	19	0.1
(1,2144)	1:6:A:VAL:HG22	1:7:A:ARG:HD3	19	0.1
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD2	19	0.1
(1,2144)	1:6:A:VAL:HG23	1:7:A:ARG:HD3	19	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG11	34	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG12	34	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG13	34	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG21	34	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG22	34	0.1
(1,2127)	1:3:A:ASP:HB2	1:6:A:VAL:HG23	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG11	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG12	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG13	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG21	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG22	34	0.1
(1,2127)	1:3:A:ASP:HB3	1:6:A:VAL:HG23	34	0.1
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD11	2	0.1
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD12	2	0.1
(1,2091)	1:42:A:GLN:HE21	1:103:A:LEU:HD13	2	0.1
(1,1922)	1:60:A:GLU:HG2	1:64:A:SER:H	29	0.1
(1,1922)	1:60:A:GLU:HG3	1:64:A:SER:H	29	0.1
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	39	0.1
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	39	0.1
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	39	0.1
(1,1819)	1:9:A:ALA:HB1	1:48:A:MET:H	40	0.1
(1,1819)	1:9:A:ALA:HB2	1:48:A:MET:H	40	0.1
(1,1819)	1:9:A:ALA:HB3	1:48:A:MET:H	40	0.1
(1,1676)	1:28:A:LEU:H	1:28:A:LEU:HG	22	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	11	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	11	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	11	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD11	17	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD12	17	0.1
(1,1557)	1:8:A:PHE:H	1:31:A:LEU:HD13	17	0.1
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD11	19	0.1
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD12	19	0.1
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD13	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD11	39	0.1
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD12	39	0.1
(1,1501)	1:51:A:ASN:HD21	1:70:A:ILE:HD13	39	0.1
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD2	32	0.1
(1,1481)	1:95:A:ASP:HA	1:96:A:LYS:HD3	32	0.1
(1,1453)	1:101:A:LYS:HG2	1:102:A:ASP:HB3	29	0.1
(1,1453)	1:101:A:LYS:HG3	1:102:A:ASP:HB3	29	0.1
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB2	36	0.1
(1,1433)	1:67:A:LYS:HD2	1:68:A:SER:HB3	36	0.1
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB2	36	0.1
(1,1433)	1:67:A:LYS:HD3	1:68:A:SER:HB3	36	0.1
(1,1304)	1:77:A:LEU:HD21	1:100:A:GLU:HG3	27	0.1
(1,1304)	1:77:A:LEU:HD22	1:100:A:GLU:HG3	27	0.1
(1,1304)	1:77:A:LEU:HD23	1:100:A:GLU:HG3	27	0.1
(1,1231)	1:31:A:LEU:HG	1:73:A:TRP:HH2	12	0.1
(1,1166)	1:70:A:ILE:HD11	1:73:A:TRP:HH2	19	0.1
(1,1166)	1:70:A:ILE:HD12	1:73:A:TRP:HH2	19	0.1
(1,1166)	1:70:A:ILE:HD13	1:73:A:TRP:HH2	19	0.1
(1,1166)	1:70:A:ILE:HD11	1:73:A:TRP:HH2	31	0.1
(1,1166)	1:70:A:ILE:HD12	1:73:A:TRP:HH2	31	0.1
(1,1166)	1:70:A:ILE:HD13	1:73:A:TRP:HH2	31	0.1
(1,1166)	1:70:A:ILE:HD11	1:73:A:TRP:HH2	33	0.1
(1,1166)	1:70:A:ILE:HD12	1:73:A:TRP:HH2	33	0.1
(1,1166)	1:70:A:ILE:HD13	1:73:A:TRP:HH2	33	0.1
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	4	0.1
(1,1105)	1:69:A:LEU:H	1:69:A:LEU:HG	27	0.1
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD21	17	0.1
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD22	17	0.1
(1,982)	1:62:A:VAL:HA	1:65:A:LEU:HD23	17	0.1
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG11	7	0.1
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG12	7	0.1
(1,965)	1:59:A:ASP:HB2	1:62:A:VAL:HG13	7	0.1
(1,947)	1:55:A:LYS:HB3	1:56:A:GLN:H	36	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	25	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	25	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	25	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD11	35	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD12	35	0.1
(1,900)	1:13:A:ASP:HA	1:53:A:ILE:HD13	35	0.1
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	6	0.1
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	6	0.1
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	16	0.1
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	16	0.1
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	16	0.1
(1,770)	1:46:A:ILE:HD11	1:50:A:VAL:H	24	0.1
(1,770)	1:46:A:ILE:HD12	1:50:A:VAL:H	24	0.1
(1,770)	1:46:A:ILE:HD13	1:50:A:VAL:H	24	0.1
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD11	30	0.1
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD12	30	0.1
(1,758)	1:46:A:ILE:HA	1:46:A:ILE:HD13	30	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	6	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	6	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	6	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	17	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	17	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	17	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG21	37	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG22	37	0.1
(1,704)	1:40:A:LEU:HG	1:44:A:THR:HG23	37	0.1
(1,668)	1:36:A:MET:HG2	1:41:A:LEU:HD11	21	0.1
(1,668)	1:36:A:MET:HG2	1:41:A:LEU:HD12	21	0.1
(1,668)	1:36:A:MET:HG2	1:41:A:LEU:HD13	21	0.1
(1,645)	1:38:A:LEU:HD21	1:78:A:ASP:H	14	0.1
(1,645)	1:38:A:LEU:HD22	1:78:A:ASP:H	14	0.1
(1,645)	1:38:A:LEU:HD23	1:78:A:ASP:H	14	0.1
(1,598)	1:37:A:THR:HB	1:76:A:LEU:HD21	29	0.1
(1,598)	1:37:A:THR:HB	1:76:A:LEU:HD22	29	0.1
(1,598)	1:37:A:THR:HB	1:76:A:LEU:HD23	29	0.1
(1,589)	1:38:A:LEU:HD21	1:42:A:GLN:HE22	36	0.1
(1,589)	1:38:A:LEU:HD22	1:42:A:GLN:HE22	36	0.1
(1,589)	1:38:A:LEU:HD23	1:42:A:GLN:HE22	36	0.1
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE1	17	0.1
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE2	17	0.1
(1,556)	1:8:A:PHE:HE1	1:36:A:MET:HE3	17	0.1
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE1	17	0.1
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE2	17	0.1
(1,556)	1:8:A:PHE:HE2	1:36:A:MET:HE3	17	0.1
(1,522)	1:34:A:ILE:HD11	1:35:A:PRO:HD3	40	0.1
(1,522)	1:34:A:ILE:HD12	1:35:A:PRO:HD3	40	0.1
(1,522)	1:34:A:ILE:HD13	1:35:A:PRO:HD3	40	0.1
(1,448)	1:31:A:LEU:HD21	1:73:A:TRP:HZ2	16	0.1
(1,448)	1:31:A:LEU:HD22	1:73:A:TRP:HZ2	16	0.1
(1,448)	1:31:A:LEU:HD23	1:73:A:TRP:HZ2	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD11	31	0.1
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD12	31	0.1
(1,441)	1:8:A:PHE:HD1	1:31:A:LEU:HD13	31	0.1
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD11	31	0.1
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD12	31	0.1
(1,441)	1:8:A:PHE:HD2	1:31:A:LEU:HD13	31	0.1
(1,406)	1:27:A:LEU:H	1:28:A:LEU:HD21	40	0.1
(1,406)	1:27:A:LEU:H	1:28:A:LEU:HD22	40	0.1
(1,406)	1:27:A:LEU:H	1:28:A:LEU:HD23	40	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	24	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	24	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	24	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD21	26	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD22	26	0.1
(1,383)	1:24:A:ALA:H	1:27:A:LEU:HD23	26	0.1
(1,313)	1:24:A:ALA:HB1	1:53:A:ILE:H	21	0.1
(1,313)	1:24:A:ALA:HB2	1:53:A:ILE:H	21	0.1
(1,313)	1:24:A:ALA:HB3	1:53:A:ILE:H	21	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	7	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	7	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	7	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	31	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	31	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	31	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB1	32	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB2	32	0.1
(1,298)	1:12:A:MET:HA	1:21:A:ALA:HB3	32	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB1	24	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB2	24	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB3	24	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB1	24	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB2	24	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB3	24	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB1	24	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB2	24	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB3	24	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB1	29	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB2	29	0.1
(1,219)	1:15:A:MET:HE1	1:24:A:ALA:HB3	29	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB1	29	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB2	29	0.1
(1,219)	1:15:A:MET:HE2	1:24:A:ALA:HB3	29	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB1	29	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB2	29	0.1
(1,219)	1:15:A:MET:HE3	1:24:A:ALA:HB3	29	0.1
(1,196)	1:9:A:ALA:HB1	1:13:A:ASP:HB2	18	0.1
(1,196)	1:9:A:ALA:HB2	1:13:A:ASP:HB2	18	0.1
(1,196)	1:9:A:ALA:HB3	1:13:A:ASP:HB2	18	0.1
(1,134)	1:9:A:ALA:HB1	1:46:A:ILE:HG21	13	0.1
(1,134)	1:9:A:ALA:HB1	1:46:A:ILE:HG22	13	0.1
(1,134)	1:9:A:ALA:HB1	1:46:A:ILE:HG23	13	0.1
(1,134)	1:9:A:ALA:HB2	1:46:A:ILE:HG21	13	0.1
(1,134)	1:9:A:ALA:HB2	1:46:A:ILE:HG22	13	0.1
(1,134)	1:9:A:ALA:HB2	1:46:A:ILE:HG23	13	0.1
(1,134)	1:9:A:ALA:HB3	1:46:A:ILE:HG21	13	0.1
(1,134)	1:9:A:ALA:HB3	1:46:A:ILE:HG22	13	0.1
(1,134)	1:9:A:ALA:HB3	1:46:A:ILE:HG23	13	0.1
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	18	0.1
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	18	0.1
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	18	0.1
(1,63)	1:5:A:VAL:HG21	1:40:A:LEU:HG	26	0.1
(1,63)	1:5:A:VAL:HG22	1:40:A:LEU:HG	26	0.1
(1,63)	1:5:A:VAL:HG23	1:40:A:LEU:HG	26	0.1
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	7	0.1
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	7	0.1
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	7	0.1
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	20	0.1
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	20	0.1
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	20	0.1
(1,60)	1:5:A:VAL:HG21	1:8:A:PHE:HB3	36	0.1
(1,60)	1:5:A:VAL:HG22	1:8:A:PHE:HB3	36	0.1
(1,60)	1:5:A:VAL:HG23	1:8:A:PHE:HB3	36	0.1
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	1	0.1
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	1	0.1
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	1	0.1
(1,58)	1:5:A:VAL:HG21	1:44:A:THR:HB	28	0.1
(1,58)	1:5:A:VAL:HG22	1:44:A:THR:HB	28	0.1
(1,58)	1:5:A:VAL:HG23	1:44:A:THR:HB	28	0.1
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE1	24	0.1
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE2	24	0.1
(1,33)	1:45:A:ARG:HD2	1:48:A:MET:HE3	24	0.1
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE1	24	0.1
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE2	24	0.1
(1,33)	1:45:A:ARG:HD3	1:48:A:MET:HE3	24	0.1

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

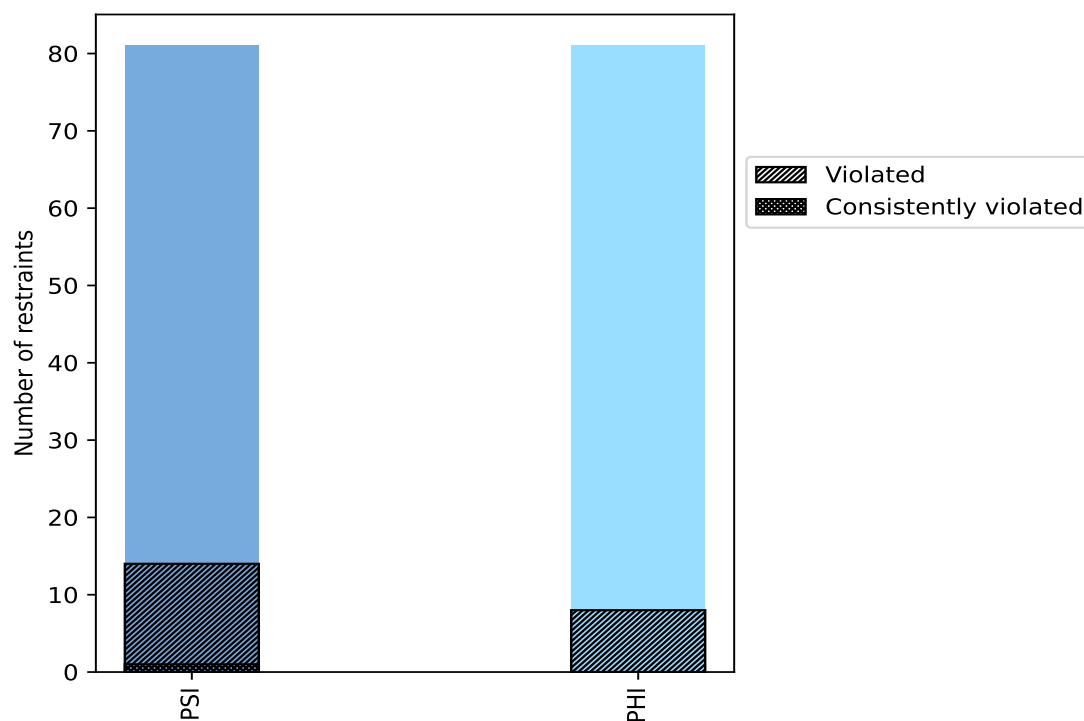
10.1 Summary of dihedral-angle violations [i](#)

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	81	50.0	14	17.3	8.6	1	1.2	0.6
PHI	81	50.0	8	9.9	4.9	0	0.0	0.0
Total	162	100.0	22	13.6	13.6	1	0.6	0.6

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

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



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

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

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

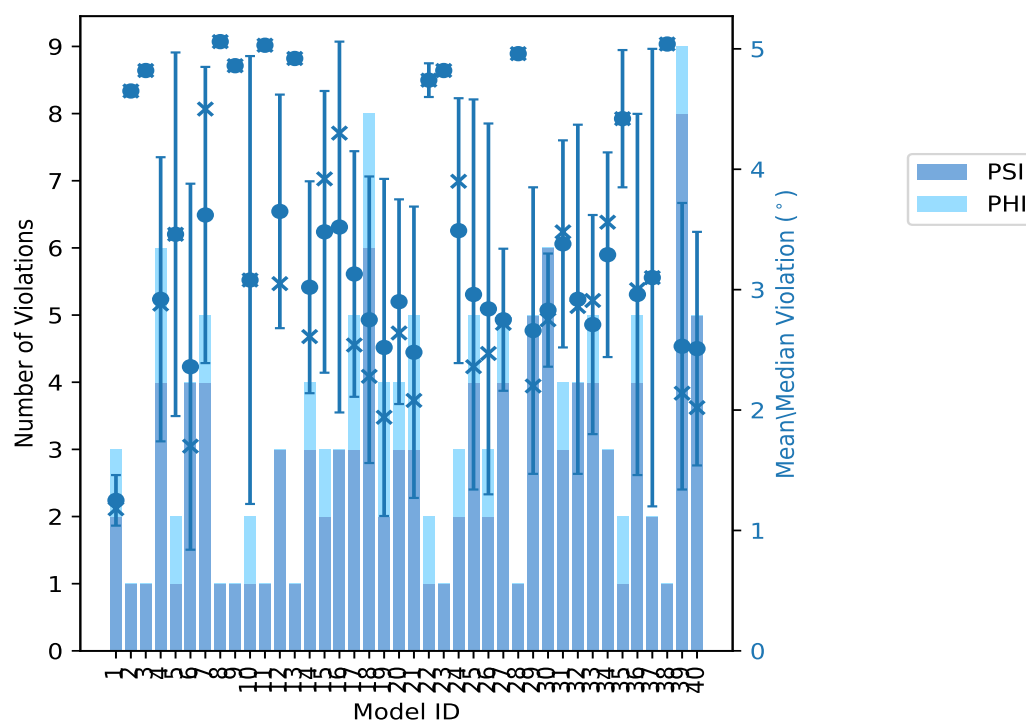
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	2	1	3	1.25	1.54	0.21	1.18
2	1	0	1	4.65	4.65	0.0	4.65
3	1	0	1	4.82	4.82	0.0	4.82
4	4	2	6	2.92	4.42	1.18	2.88
5	1	1	2	3.46	4.97	1.51	3.46
6	4	0	4	2.36	4.95	1.52	1.7
7	4	1	5	3.62	4.77	1.23	4.5
8	1	0	1	5.06	5.06	0.0	5.06
9	1	0	1	4.86	4.86	0.0	4.86
10	1	1	2	3.08	4.94	1.86	3.08
11	1	0	1	5.03	5.03	0.0	5.03
12	3	0	3	3.65	5.01	0.97	3.05
13	1	0	1	4.92	4.92	0.0	4.92
14	3	1	4	3.02	4.54	0.88	2.61
15	2	1	3	3.48	4.63	1.17	3.92
16	3	0	3	3.52	4.89	1.54	4.3
17	3	2	5	3.13	5.04	1.02	2.54
18	6	2	8	2.75	4.52	1.19	2.28
19	2	2	4	2.52	4.89	1.4	1.94
20	3	1	4	2.9	4.29	0.85	2.64
21	3	2	5	2.48	4.78	1.21	2.08
22	1	1	2	4.74	4.88	0.14	4.74
23	1	0	1	4.82	4.82	0.0	4.82
24	2	1	3	3.49	4.58	1.1	3.9
25	4	1	5	2.96	4.98	1.62	2.36
26	2	1	3	2.84	4.89	1.54	2.47
27	4	1	5	2.75	3.75	0.59	2.72
28	1	0	1	4.96	4.96	0.0	4.96
29	5	0	5	2.66	4.87	1.19	2.2
30	6	0	6	2.83	3.5	0.47	2.75
31	3	1	4	3.38	4.47	0.86	3.48
32	4	0	4	2.92	4.93	1.45	2.86
33	4	1	5	2.71	4.01	0.91	2.91
34	3	0	3	3.29	4.18	0.85	3.56
35	1	1	2	4.42	4.98	0.57	4.42
36	4	1	5	2.96	4.95	1.5	3.0
37	2	0	2	3.1	5.0	1.9	3.1
38	1	0	1	5.04	5.04	0.0	5.04

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	8	1	9	2.53	4.82	1.19	2.14
40	5	0	5	2.51	4.11	0.97	2.02

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
4	3	7	1	2.5
0	0	0	2	5.0
2	2	4	3	7.5
0	0	0	4	10.0

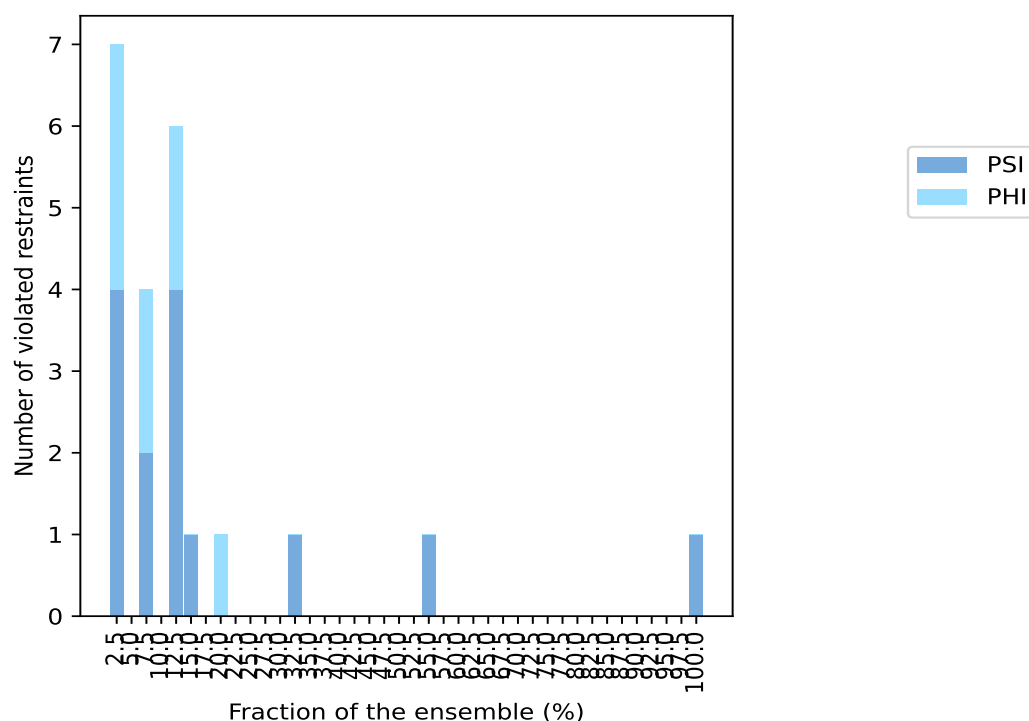
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
4	2	6	5	12.5
1	0	1	6	15.0
0	0	0	7	17.5
0	1	1	8	20.0
0	0	0	9	22.5
0	0	0	10	25.0
0	0	0	11	27.5
0	0	0	12	30.0
1	0	1	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	0	0	20	50.0
0	0	0	21	52.5
1	0	1	22	55.0
0	0	0	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	0	0	28	70.0
0	0	0	29	72.5
0	0	0	30	75.0
0	0	0	31	77.5
0	0	0	32	80.0
0	0	0	33	82.5
0	0	0	34	85.0
0	0	0	35	87.5
0	0	0	36	90.0
0	0	0	37	92.5
0	0	0	38	95.0
0	0	0	39	97.5
1	0	1	40	100.0

¹ Number of models with violations

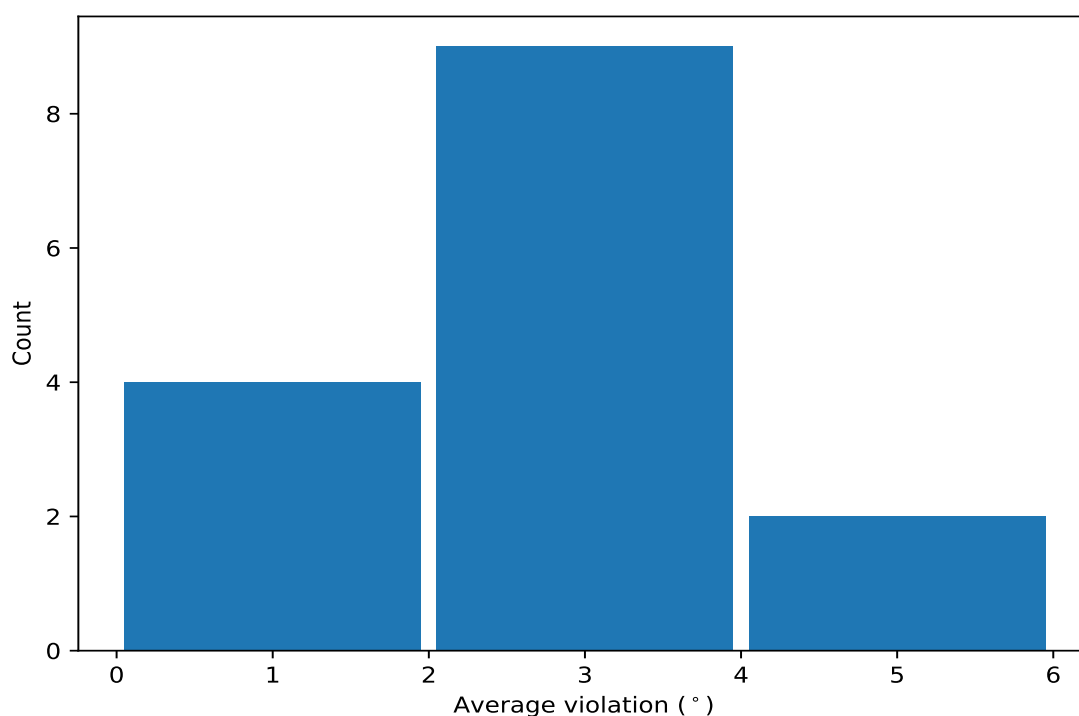
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

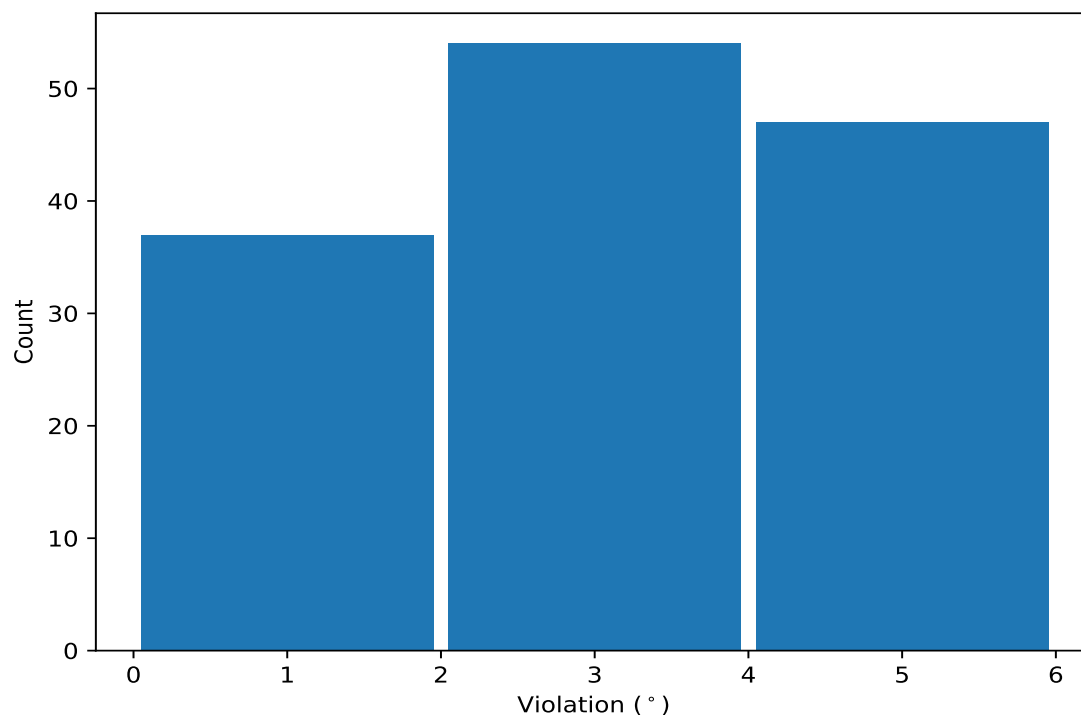
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	40	4.34	0.87	4.72
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	22	2.32	0.88	2.18
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	13	3.34	1.04	3.31
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	8	2.25	1.03	2.12
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	6	2.92	0.76	2.83
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	5	4.82	0.19	4.88
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	5	2.94	0.89	2.8
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	5	2.85	0.84	2.36
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	5	2.22	0.98	1.95
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	5	1.98	0.45	2.14
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	5	1.82	0.43	1.88
(1,38)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ALA:N	3	2.47	1.38	1.58
(1,47)	1:25:A:LEU:C	1:26:A:ASP:N	1:26:A:ASP:CA	1:26:A:ASP:C	3	2.16	0.68	2.44
(1,157)	1:101:A:LYS:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	3	1.83	0.37	1.69
(1,142)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:GLY:N	3	1.67	0.41	1.93

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 (°)
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	8	5.06
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	38	5.04
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	17	5.04
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	11	5.03
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	12	5.01
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	37	5.0
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	25	4.98
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	35	4.98
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	5	4.97
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	28	4.96
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	6	4.95
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	36	4.95
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	10	4.94
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	32	4.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	13	4.92
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	16	4.89
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	19	4.89
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	26	4.89
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	22	4.88
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	29	4.87
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	9	4.86
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	3	4.82
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	23	4.82
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	39	4.82
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	25	4.79
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	21	4.78
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	7	4.77
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	2	4.65
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	15	4.63
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	22	4.6
(1,131)	1:72:A:SER:C	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	24	4.58
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	14	4.54
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	7	4.53
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	18	4.52
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	7	4.5
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	31	4.47
(1,38)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ALA:N	4	4.42
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	16	4.3
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	20	4.29
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	4	4.27
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	36	4.23
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	34	4.18
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	40	4.11
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	18	4.08
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	39	4.03
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	18	4.02
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	33	4.01
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	15	3.92
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	24	3.9
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	35	3.85
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	27	3.75
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	31	3.69
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	34	3.56
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	30	3.5
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	32	3.5
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	39	3.41
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	17	3.32
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	30	3.31
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	31	3.28
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	33	3.25
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	40	3.06
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	12	3.05
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	36	3.0
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	4	2.96
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	33	2.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:2:A:GLU:N	1:2:A:GLU:CA	1:2:A:GLU:C	1:3:A:ASP:N	12	2.88
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	29	2.86
(1,109)	1:61:A:GLU:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	27	2.85
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	30	2.84
(1,47)	1:25:A:LEU:C	1:26:A:ASP:N	1:26:A:ASP:CA	1:26:A:ASP:C	20	2.82
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	4	2.8
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	27	2.72
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	30	2.66
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	14	2.61
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	30	2.61
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	14	2.61
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	17	2.54
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	27	2.52
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	21	2.49
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	26	2.47
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	7	2.46
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	20	2.46
(1,47)	1:25:A:LEU:C	1:26:A:ASP:N	1:26:A:ASP:CA	1:26:A:ASP:C	17	2.44
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	25	2.36
(1,157)	1:101:A:LYS:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	14	2.34
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	17	2.29
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	18	2.28
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	18	2.27
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	32	2.23
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	39	2.21
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	29	2.2
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	19	2.2
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	18	2.16
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	34	2.14
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	39	2.14
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	31	2.09
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	30	2.09
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	21	2.08
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	4	2.08
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	20	2.04
(1,44)	1:24:A:ALA:N	1:24:A:ALA:CA	1:24:A:ALA:C	1:25:A:LEU:N	40	2.02
(1,142)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:GLY:N	40	1.98
(1,18)	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	1:11:A:LYS:N	24	1.98
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	5	1.95
(1,142)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:GLY:N	27	1.93
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	15	1.88
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	33	1.88
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	6	1.84
(1,134)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LYS:N	39	1.83
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	7	1.82
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	39	1.8
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	29	1.77
(1,157)	1:101:A:LYS:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	19	1.69
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	18	1.59
(1,38)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ALA:N	29	1.58
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	21	1.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	6	1.56
(1,132)	1:73:A:TRP:N	1:73:A:TRP:CA	1:73:A:TRP:C	1:74:A:LYS:N	1	1.54
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	36	1.54
(1,42)	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1:24:A:ALA:N	33	1.52
(1,157)	1:101:A:LYS:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	21	1.46
(1,38)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ALA:N	39	1.42
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	25	1.39
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	40	1.38
(1,24)	1:13:A:ASP:N	1:13:A:ASP:CA	1:13:A:ASP:C	1:14:A:LYS:N	16	1.36
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	19	1.31
(1,139)	1:76:A:LEU:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	25	1.28
(1,47)	1:25:A:LEU:C	1:26:A:ASP:N	1:26:A:ASP:CA	1:26:A:ASP:C	10	1.22
(1,112)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:SER:N	37	1.2
(1,120)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:SER:N	1	1.18
(1,17)	1:9:A:ALA:C	1:10:A:LYS:N	1:10:A:LYS:CA	1:10:A:LYS:C	26	1.17
(1,128)	1:71:A:LYS:N	1:71:A:LYS:CA	1:71:A:LYS:C	1:72:A:SER:N	18	1.11
(1,142)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:GLY:N	39	1.09
(1,108)	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	1:62:A:VAL:N	6	1.09
(1,129)	1:71:A:LYS:C	1:72:A:SER:N	1:72:A:SER:CA	1:72:A:SER:C	36	1.06
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	1	1.04
(1,27)	1:14:A:LYS:C	1:15:A:MET:N	1:15:A:MET:CA	1:15:A:MET:C	4	1.02
(1,26)	1:14:A:LYS:N	1:14:A:LYS:CA	1:14:A:LYS:C	1:15:A:MET:N	32	1.02