



Full wwPDB NMR Structure Validation Report ⓘ

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Title : CSP1-f11
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

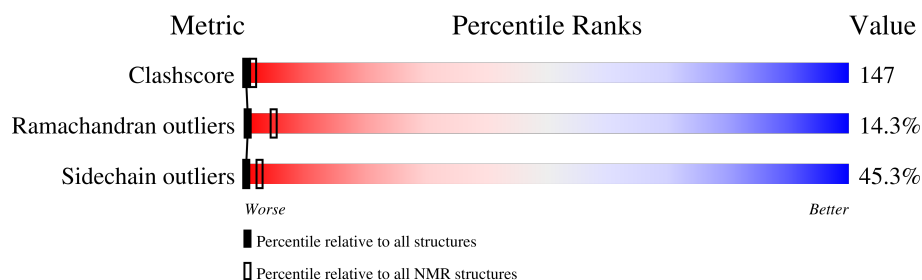
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	17	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:10, A:12-A:17 (15)	0.19	18

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 330 atoms, of which 172 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Competence-stimulating peptide type 1.

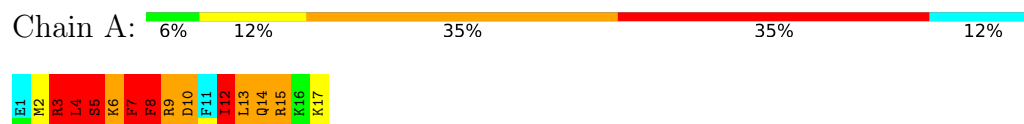
Mol	Chain	Residues	Atoms							Trace
1	A	17	Total	C	H	N	O	S		0
			330	103	172	30	24	1		

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: Competence-stimulating peptide type 1

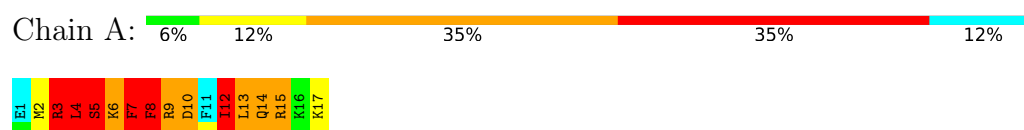


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: Competence-stimulating peptide type 1



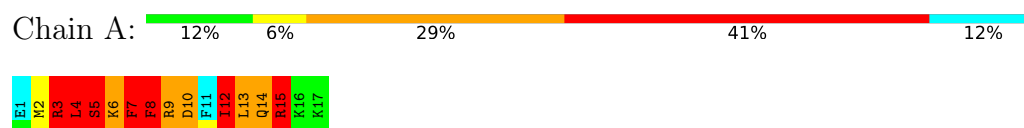
4.2.2 Score per residue for model 2

- Molecule 1: Competence-stimulating peptide type 1



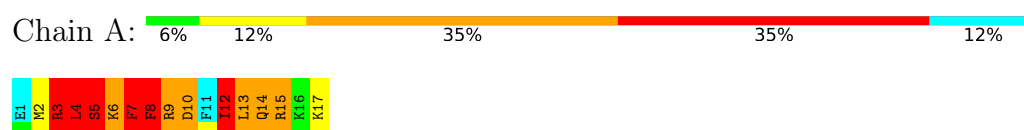
4.2.3 Score per residue for model 3

- Molecule 1: Competence-stimulating peptide type 1



4.2.4 Score per residue for model 4

- Molecule 1: Competence-stimulating peptide type 1



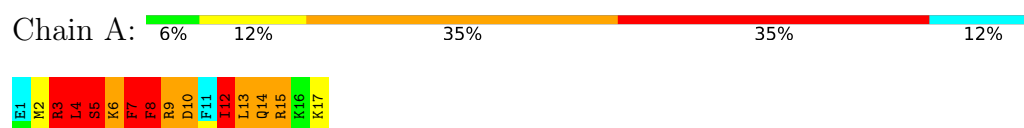
4.2.5 Score per residue for model 5

- Molecule 1: Competence-stimulating peptide type 1



4.2.6 Score per residue for model 6

- Molecule 1: Competence-stimulating peptide type 1



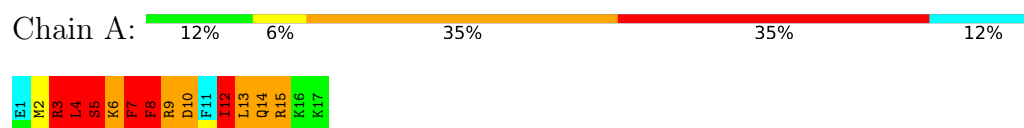
4.2.7 Score per residue for model 7

- Molecule 1: Competence-stimulating peptide type 1



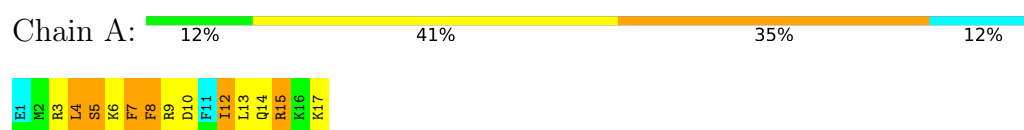
4.2.8 Score per residue for model 8

- Molecule 1: Competence-stimulating peptide type 1



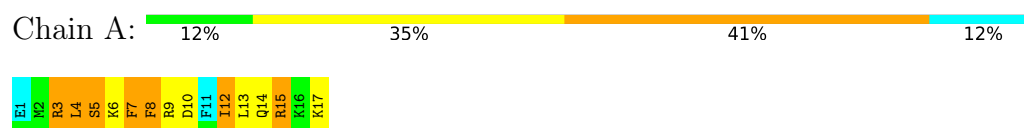
4.2.9 Score per residue for model 9

- Molecule 1: Competence-stimulating peptide type 1



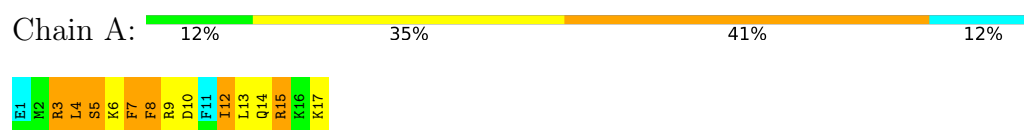
4.2.10 Score per residue for model 10

- Molecule 1: Competence-stimulating peptide type 1



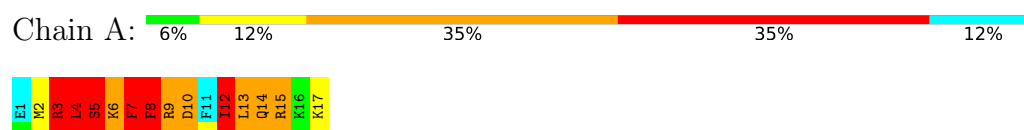
4.2.11 Score per residue for model 11

- Molecule 1: Competence-stimulating peptide type 1



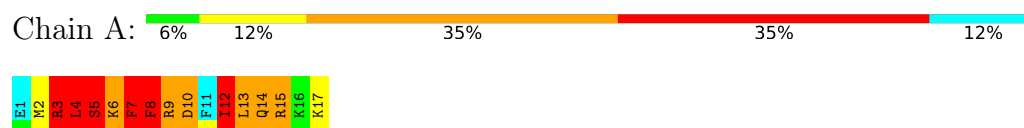
4.2.12 Score per residue for model 12

- Molecule 1: Competence-stimulating peptide type 1



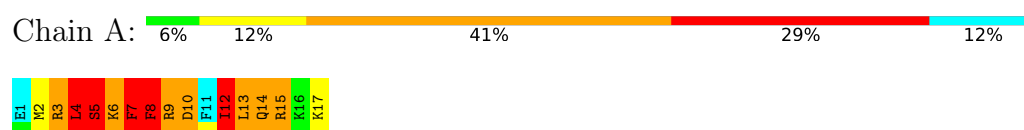
4.2.13 Score per residue for model 13

- Molecule 1: Competence-stimulating peptide type 1



4.2.14 Score per residue for model 14

- Molecule 1: Competence-stimulating peptide type 1



4.2.15 Score per residue for model 15

- Molecule 1: Competence-stimulating peptide type 1



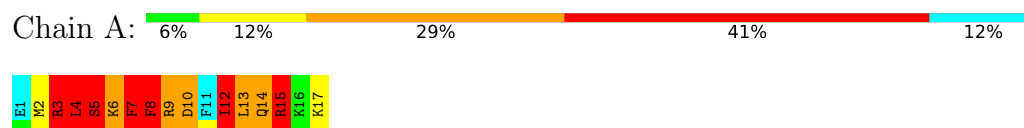
4.2.16 Score per residue for model 16

- Molecule 1: Competence-stimulating peptide type 1



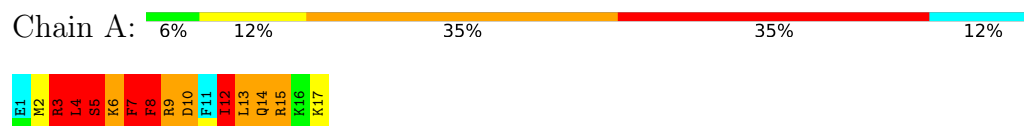
4.2.17 Score per residue for model 17

- Molecule 1: Competence-stimulating peptide type 1



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Competence-stimulating peptide type 1



4.2.19 Score per residue for model 19

- Molecule 1: Competence-stimulating peptide type 1



4.2.20 Score per residue for model 20

- Molecule 1: Competence-stimulating peptide type 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	149
Number of shifts mapped to atoms	149
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DPN

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	2.90±0.01	14±0/138 (10.0± 0.3%)	2.62±0.03	14±1/175 (8.3± 0.3%)
All	All	2.90	277/2760 (10.0%)	2.62	290/3500 (8.3%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	20

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	PHE	CA-C	-12.93	1.35	1.52	5	20
1	A	7	PHE	CA-C	-8.13	1.41	1.52	9	20
1	A	8	PHE	C-O	-7.84	1.14	1.24	15	20
1	A	9	ARG	N-CA	-7.76	1.35	1.46	19	20
1	A	8	PHE	CB-CG	-7.32	1.33	1.50	12	20
1	A	9	ARG	CA-C	-6.78	1.43	1.52	5	20
1	A	3	ARG	CA-C	-6.34	1.44	1.52	3	20
1	A	4	LEU	CA-C	-6.32	1.44	1.52	2	20
1	A	10	ASP	N-CA	-6.29	1.34	1.46	4	20
1	A	4	LEU	N-CA	-6.26	1.38	1.46	20	20
1	A	10	ASP	CA-CB	-6.09	1.41	1.53	19	20
1	A	8	PHE	N-CA	-5.86	1.38	1.46	12	20
1	A	13	LEU	CA-C	-5.46	1.47	1.52	19	20
1	A	7	PHE	N-CA	-5.18	1.39	1.46	7	17

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	6	LYS	N-CA-C	-13.22	97.20	113.20	13	20
1	A	8	PHE	N-CA-C	-9.36	99.44	112.45	5	20
1	A	7	PHE	CA-CB-CG	8.19	121.99	113.80	13	20
1	A	9	ARG	N-CA-C	-7.44	104.08	113.01	15	20
1	A	8	PHE	CB-CA-C	-7.36	96.20	110.11	10	20
1	A	4	LEU	N-CA-C	-7.10	103.48	111.14	12	20
1	A	7	PHE	CB-CA-C	-7.00	96.48	110.42	11	20
1	A	8	PHE	N-CA-CB	6.89	120.52	110.26	5	20
1	A	4	LEU	O-C-N	6.79	129.07	122.07	5	20
1	A	15	ARG	N-CA-C	-6.64	105.31	113.41	6	20
1	A	7	PHE	N-CA-C	6.17	123.94	110.80	3	20
1	A	14	GLN	N-CA-C	-5.93	105.31	112.54	11	20
1	A	16	LYS	N-CA-C	-5.56	106.08	112.86	15	5
1	A	4	LEU	CA-C-N	5.19	131.45	121.54	9	20
1	A	4	LEU	C-N-CA	5.19	131.45	121.54	9	20
1	A	3	ARG	N-CA-C	-5.06	108.13	114.56	2	5

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	7	PHE	Sidechain	20

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	138	155	155	37±22
All	All	2760	3100	2325	747

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 147.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:CA	1:A:12:ILE:HD11	0.97	1.89	4	15
1:A:8:PHE:CB	1:A:12:ILE:HD11	0.96	1.91	14	15
1:A:4:LEU:HD12	1:A:8:PHE:CE2	0.83	2.09	20	15
1:A:4:LEU:C	1:A:7:PHE:HB2	0.80	2.02	12	15
1:A:8:PHE:HA	1:A:12:ILE:HD11	0.77	1.57	1	15
1:A:12:ILE:HG22	1:A:17:LYS:HG2	0.74	1.59	20	5
1:A:2:MET:HE3	1:A:3:ARG:H	0.72	1.44	13	15
1:A:8:PHE:C	1:A:10:ASP:N	0.69	2.49	18	15
1:A:4:LEU:HB3	1:A:7:PHE:CD1	0.69	2.23	3	15
1:A:4:LEU:HD12	1:A:8:PHE:CD2	0.67	2.25	7	15
1:A:12:ILE:HD13	1:A:13:LEU:CD2	0.67	2.20	19	15
1:A:2:MET:HE3	1:A:3:ARG:N	0.66	2.06	13	15
1:A:12:ILE:CD1	1:A:13:LEU:HG	0.66	2.20	15	15
1:A:12:ILE:N	1:A:12:ILE:HD12	0.64	2.06	12	15
1:A:8:PHE:C	1:A:10:ASP:H	0.63	2.00	7	15
1:A:4:LEU:O	1:A:6:LYS:N	0.63	2.32	15	15
1:A:12:ILE:HD12	1:A:13:LEU:HG	0.60	1.73	7	15
1:A:8:PHE:HB2	1:A:13:LEU:HD11	0.59	1.73	7	15
1:A:7:PHE:CD2	1:A:7:PHE:C	0.57	2.80	19	15
1:A:8:PHE:HA	1:A:12:ILE:CD1	0.57	2.27	3	15
1:A:5:SER:C	1:A:7:PHE:H	0.57	2.05	3	15
1:A:5:SER:C	1:A:7:PHE:N	0.57	2.62	15	15
1:A:12:ILE:HD12	1:A:13:LEU:N	0.56	2.15	20	15
1:A:12:ILE:CD1	1:A:13:LEU:CD2	0.56	2.84	19	15
1:A:8:PHE:CE1	1:A:9:ARG:HG2	0.55	2.36	14	15
1:A:7:PHE:C	1:A:10:ASP:H	0.55	2.09	15	15
1:A:4:LEU:O	1:A:7:PHE:HB2	0.53	2.02	13	15
1:A:5:SER:CB	1:A:8:PHE:CZ	0.53	2.92	3	15
1:A:8:PHE:HB3	1:A:12:ILE:HD11	0.51	1.79	3	15
1:A:7:PHE:C	1:A:7:PHE:HD2	0.50	2.14	13	15
1:A:12:ILE:N	1:A:12:ILE:CD1	0.50	2.71	14	6
1:A:12:ILE:CD1	1:A:12:ILE:N	0.49	2.72	20	9
1:A:5:SER:O	1:A:9:ARG:HB2	0.48	2.08	3	15
1:A:8:PHE:CG	1:A:9:ARG:N	0.48	2.79	7	15
1:A:4:LEU:C	1:A:7:PHE:CB	0.48	2.84	1	15
1:A:8:PHE:CA	1:A:12:ILE:CD1	0.47	2.80	6	8
1:A:4:LEU:HB2	1:A:8:PHE:CD2	0.47	2.44	20	15
1:A:4:LEU:O	1:A:7:PHE:N	0.47	2.48	8	15
1:A:12:ILE:HD13	1:A:13:LEU:HD21	0.46	1.85	16	15
1:A:8:PHE:HA	1:A:12:ILE:CG1	0.45	2.40	19	15
1:A:12:ILE:CD1	1:A:13:LEU:CG	0.45	2.94	16	15
1:A:4:LEU:HB2	1:A:8:PHE:CE2	0.45	2.47	18	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:SER:HB2	1:A:8:PHE:CZ	0.45	2.47	12	14
1:A:12:ILE:HD12	1:A:12:ILE:C	0.45	2.36	3	15
1:A:13:LEU:C	1:A:15:ARG:N	0.44	2.73	15	7
1:A:4:LEU:CD1	1:A:8:PHE:CE2	0.44	2.95	20	14
1:A:8:PHE:CD2	1:A:8:PHE:N	0.43	2.86	14	15
1:A:5:SER:CA	1:A:8:PHE:CE2	0.43	3.02	3	15
1:A:2:MET:HE3	1:A:2:MET:CA	0.42	2.43	14	6
1:A:12:ILE:CD1	1:A:12:ILE:C	0.42	2.92	8	11
1:A:5:SER:N	1:A:8:PHE:CE2	0.42	2.88	12	15
1:A:6:LYS:O	1:A:10:ASP:CB	0.42	2.68	1	15
1:A:8:PHE:CD1	1:A:9:ARG:N	0.41	2.89	3	13
1:A:2:MET:HE2	1:A:4:LEU:HD21	0.41	1.93	12	4
1:A:2:MET:HE2	1:A:4:LEU:CG	0.40	2.46	19	2
1:A:2:MET:HE2	1:A:4:LEU:HG	0.40	1.93	19	3

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	14/17 (82%)	11±1 (77±4%)	1±1 (9±4%)	2±0 (14±0%)	05
All	All	280/340 (82%)	215 (77%)	25 (9%)	40 (14%)	05

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	5	SER	20
1	A	12	ILE	20

6.3.2 Protein sidechains

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	15/16 (94%)	8±1 (55±3%)	7±1 (45±3%)	0	2
All	All	300/320 (94%)	164 (55%)	136 (45%)	0	2

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

Mol	Chain	Res	Type	Models (Total)
1	A	4	LEU	20
1	A	5	SER	20
1	A	8	PHE	20
1	A	12	ILE	20
1	A	15	ARG	20
1	A	17	LYS	18
1	A	3	ARG	16
1	A	2	MET	1
1	A	16	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 54% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shiftFile_1*

7.1.1 Bookkeeping

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

Total number of shifts	149
Number of shifts mapped to atoms	149
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 54%, i.e. 141 atoms were assigned a chemical shift out of a possible 260. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	48/75 (64%)	28/30 (93%)	14/30 (47%)	6/15 (40%)
Sidechain	88/165 (53%)	74/105 (70%)	14/47 (30%)	0/13 (0%)
Aromatic	5/20 (25%)	5/10 (50%)	0/10 (0%)	0/0 (—%)
Overall	141/260 (54%)	107/145 (74%)	28/87 (32%)	6/28 (21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 141 atoms were assigned a chemical shift out of a possible 272. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	48/80 (60%)	28/32 (88%)	14/32 (44%)	6/16 (38%)
Sidechain	88/172 (51%)	74/109 (68%)	14/50 (28%)	0/13 (0%)
Aromatic	5/20 (25%)	5/10 (50%)	0/10 (0%)	0/0 (—%)
Overall	141/272 (52%)	107/151 (71%)	28/92 (30%)	6/29 (21%)

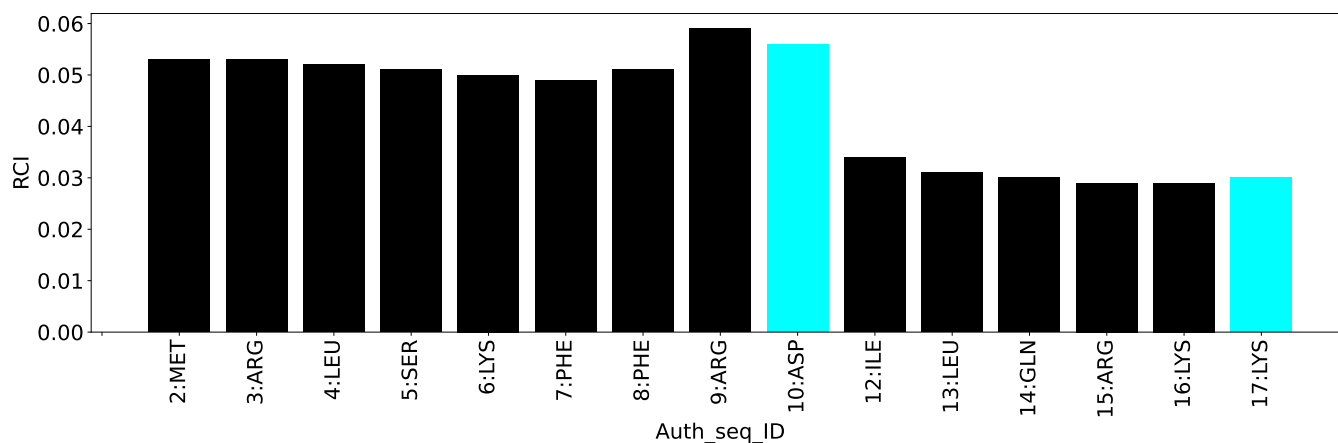
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	592
Intra-residue ($ i-j =0$)	162
Sequential ($ i-j =1$)	163
Medium range ($ i-j >1$ and $ i-j <5$)	235
Long range ($ i-j \geq 5$)	26
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	0
Total dihedral-angle restraints	22
Number of unmapped restraints	0
Number of restraints per residue	36.1
Number of long range restraints per residue ¹	1.5

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)	46.5	0.2
0.2-0.5 (Medium)	176.7	0.5
>0.5 (Large)	49.0	2.07

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)	5.0	9.07
10.0-20.0 (Medium)	4.0	18.21
>20.0 (Large)	3.0	63.2

9 Distance violation analysis ⓘ

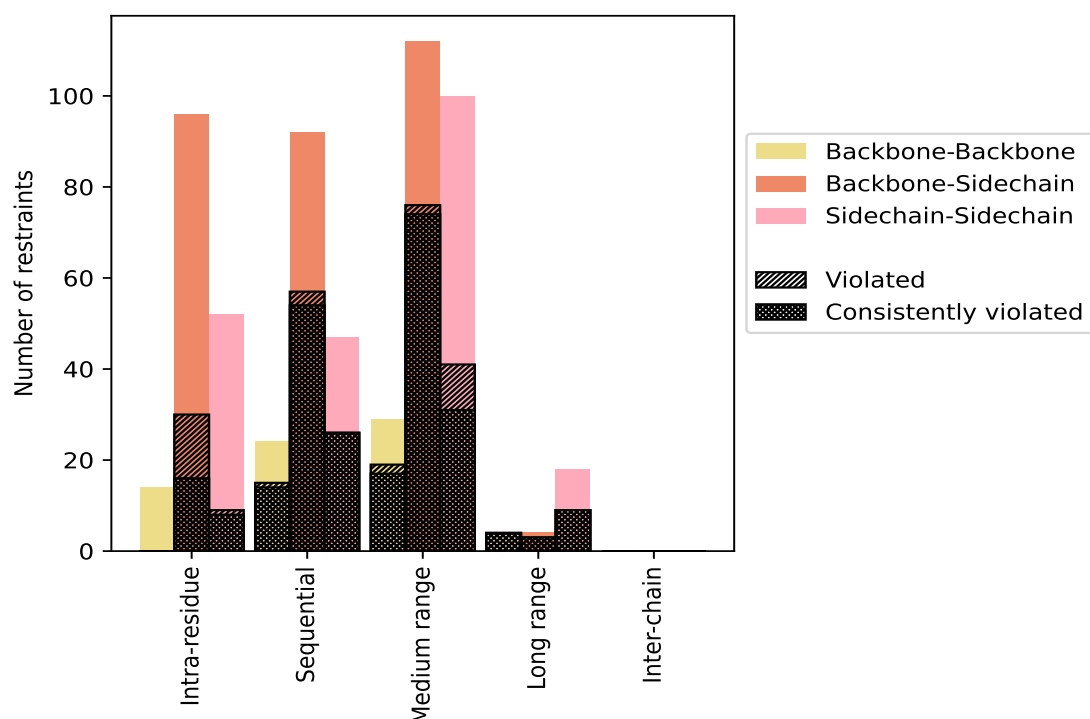
9.1 Summary of distance violations ⓘ

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)	162	27.4	39	24.1	6.6	24	14.8	4.1
Backbone-Backbone	14	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	96	16.2	30	31.2	5.1	16	16.7	2.7
Sidechain-Sidechain	52	8.8	9	17.3	1.5	8	15.4	1.4
Sequential (i-j =1)	163	27.5	98	60.1	16.6	94	57.7	15.9
Backbone-Backbone	24	4.1	15	62.5	2.5	14	58.3	2.4
Backbone-Sidechain	92	15.5	57	62.0	9.6	54	58.7	9.1
Sidechain-Sidechain	47	7.9	26	55.3	4.4	26	55.3	4.4
Medium range (i-j >1 & i-j <5)	235	39.7	130	55.3	22.0	116	49.4	19.6
Backbone-Backbone	29	4.9	19	65.5	3.2	17	58.6	2.9
Backbone-Sidechain	106	17.9	70	66.0	11.8	68	64.2	11.5
Sidechain-Sidechain	100	16.9	41	41.0	6.9	31	31.0	5.2
Long range (i-j ≥5)	26	4.4	16	61.5	2.7	16	61.5	2.7
Backbone-Backbone	4	0.7	4	100.0	0.7	4	100.0	0.7
Backbone-Sidechain	4	0.7	3	75.0	0.5	3	75.0	0.5
Sidechain-Sidechain	18	3.0	9	50.0	1.5	9	50.0	1.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	1.0	6	100.0	1.0	6	100.0	1.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	592	100.0	289	48.8	48.8	256	43.2	43.2
Backbone-Backbone	71	12.0	38	53.5	6.4	35	49.3	5.9
Backbone-Sidechain	304	51.4	166	54.6	28.0	147	48.4	24.8
Sidechain-Sidechain	217	36.7	85	39.2	14.4	74	34.1	12.5

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	30	97	131	16	0	274	0.45	2.07	0.35	0.37
2	26	98	132	16	0	272	0.45	1.9	0.35	0.37
3	28	98	131	16	0	273	0.45	2.07	0.35	0.37
4	28	97	130	16	0	271	0.46	2.07	0.35	0.37
5	30	95	127	16	0	268	0.46	2.06	0.36	0.37
6	30	97	130	16	0	273	0.45	1.88	0.35	0.37
7	29	97	132	16	0	274	0.45	2.04	0.36	0.37
8	30	97	131	16	0	274	0.45	2.07	0.35	0.37
9	28	98	130	16	0	272	0.45	1.89	0.35	0.37
10	28	98	131	16	0	273	0.45	2.06	0.36	0.37

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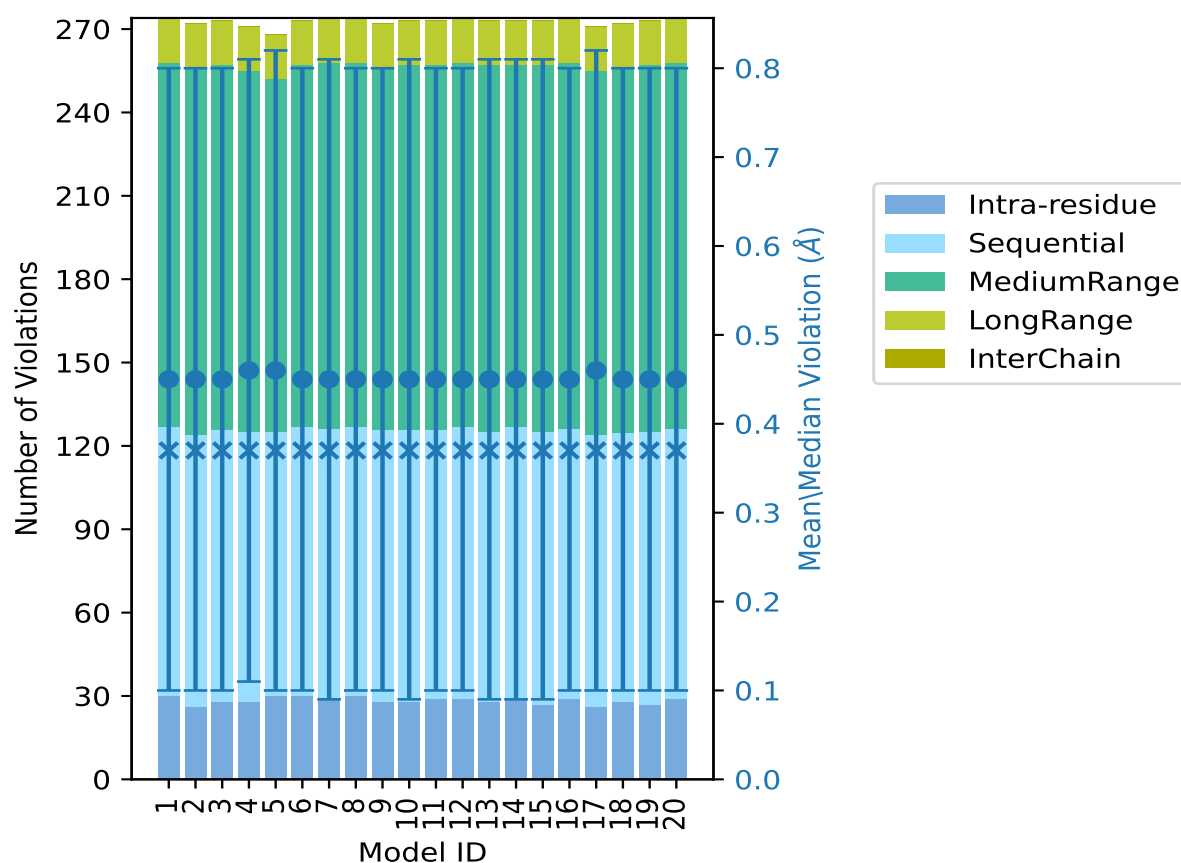
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	29	97	131	16	0	273	0.45	1.95	0.35	0.37
12	29	98	131	16	0	274	0.45	1.88	0.35	0.37
13	28	97	132	16	0	273	0.45	2.06	0.36	0.37
14	29	98	130	16	0	273	0.45	2.06	0.36	0.37
15	27	98	132	16	0	273	0.45	2.02	0.36	0.37
16	29	97	132	16	0	274	0.45	1.9	0.35	0.37
17	26	98	131	16	0	271	0.46	2.06	0.36	0.37
18	28	97	131	16	0	272	0.45	1.96	0.35	0.37
19	27	98	132	16	0	273	0.45	1.88	0.35	0.37
20	29	97	132	16	0	274	0.45	1.89	0.35	0.37

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

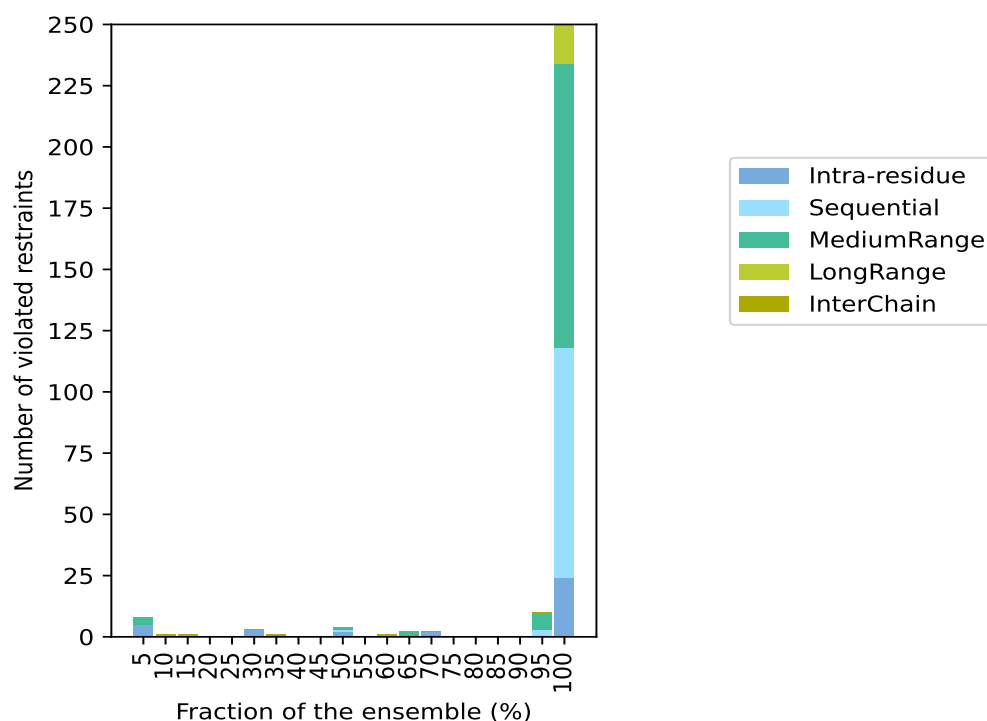
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 303(IR:123, SQ:65, MR:105, LR:10, IC:0) restraints are not 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	%
5	0	3	0	0	8	1	5.0
1	0	0	0	0	1	2	10.0
1	0	0	0	0	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
3	0	0	0	0	3	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
2	1	1	0	0	4	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	0	0	1	12	60.0
0	0	2	0	0	2	13	65.0
2	0	0	0	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	3	7	0	0	10	19	95.0
24	94	116	16	0	250	20	100.0

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

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

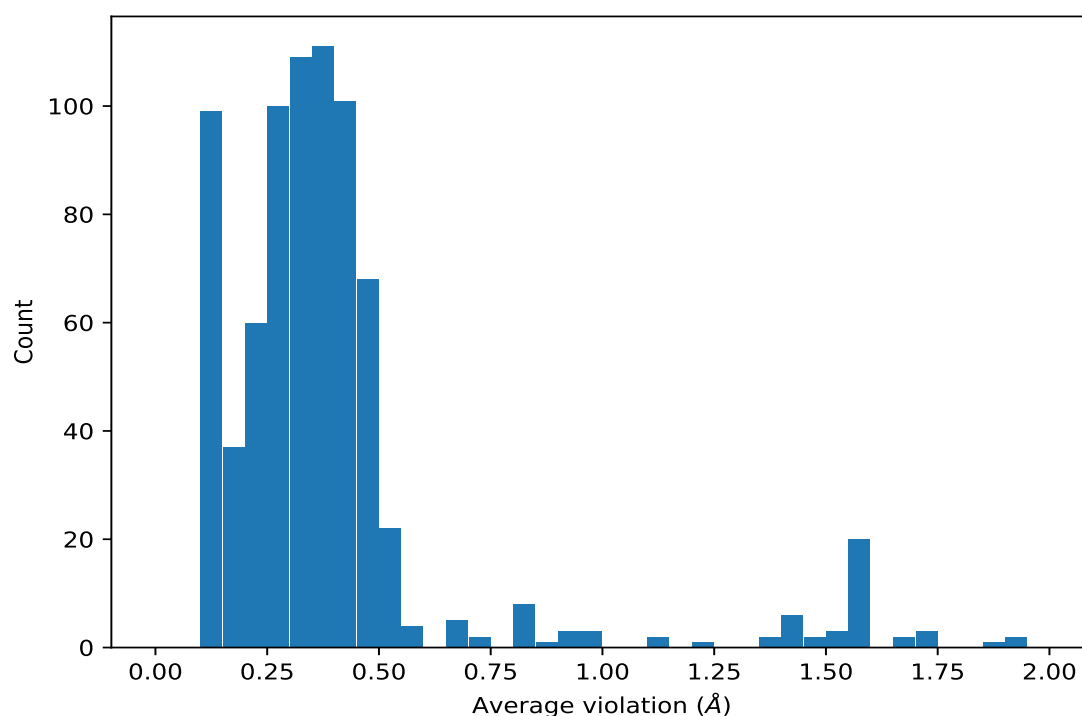
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	20	1.91	0.18	2.03
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	20	1.91	0.18	2.03
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	20	1.89	0.01	1.89
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	20	1.72	0.01	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	20	1.72	0.01	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.72	0.01	1.72
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	20	1.68	0.0	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	20	1.68	0.0	1.68
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	20	1.59	0.01	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	20	1.59	0.01	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	20	1.57	0.0	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	20	1.57	0.0	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.57	0.0	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	20	1.57	0.0	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	20	1.57	0.0	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.57	0.0	1.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	20	1.56	0.01	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	20	1.56	0.01	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	20	1.56	0.01	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	20	1.56	0.01	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	20	1.56	0.01	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	20	1.56	0.01	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	20	1.56	0.01	1.56
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	20	1.53	0.0	1.53
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	20	1.5	0.0	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	20	1.5	0.0	1.5
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	20	1.46	0.0	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	20	1.46	0.0	1.46
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	20	1.45	0.0	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	20	1.45	0.0	1.45
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	20	1.42	0.01	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	20	1.42	0.0	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	20	1.42	0.0	1.42
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	20	1.41	0.01	1.41
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	20	1.39	0.01	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	20	1.39	0.01	1.38
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	20	1.22	0.01	1.22
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	20	1.13	0.0	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	20	1.13	0.0	1.13
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	20	0.99	0.01	1.0
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	20	0.96	0.0	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	20	0.96	0.0	0.96
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	20	0.94	0.01	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	20	0.94	0.01	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	20	0.94	0.01	0.93
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	20	0.86	0.01	0.86
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	20	0.84	0.01	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	20	0.84	0.01	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	20	0.84	0.01	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	20	0.84	0.01	0.84
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	20	0.82	0.02	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	20	0.8	0.0	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	20	0.8	0.0	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	20	0.8	0.0	0.8
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	20	0.74	0.01	0.74
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	20	0.72	0.02	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	20	0.7	0.01	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	20	0.7	0.01	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	20	0.7	0.01	0.71
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	20	0.7	0.02	0.69
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	20	0.65	0.02	0.65
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	20	0.59	0.0	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	20	0.59	0.0	0.59
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	20	0.55	0.02	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	20	0.55	0.0	0.55
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	20	0.53	0.0	0.53
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	20	0.52	0.0	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	20	0.52	0.01	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	20	0.52	0.01	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	20	0.52	0.01	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	20	0.52	0.01	0.52
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	20	0.51	0.0	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	20	0.51	0.0	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	20	0.51	0.0	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	20	0.51	0.0	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	20	0.51	0.0	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	20	0.51	0.0	0.51
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	20	0.5	0.0	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	20	0.5	0.0	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	20	0.5	0.0	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	20	0.5	0.0	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	20	0.5	0.0	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	20	0.5	0.0	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	20	0.5	0.0	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	20	0.5	0.0	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	20	0.5	0.0	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	20	0.5	0.0	0.5
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	20	0.49	0.0	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	20	0.49	0.0	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	20	0.49	0.0	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	20	0.49	0.0	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	20	0.48	0.0	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	20	0.48	0.0	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	20	0.48	0.0	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	20	0.48	0.0	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	20	0.48	0.0	0.48
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	20	0.48	0.04	0.47
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	20	0.48	0.04	0.47
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	20	0.48	0.04	0.47
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	20	0.48	0.04	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	20	0.47	0.02	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	20	0.47	0.02	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	20	0.47	0.02	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	20	0.47	0.02	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	20	0.47	0.02	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	20	0.47	0.02	0.48
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	20	0.47	0.0	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	20	0.47	0.0	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	20	0.47	0.0	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	20	0.47	0.0	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	20	0.47	0.0	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	20	0.47	0.0	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	20	0.46	0.01	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	20	0.46	0.01	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	20	0.46	0.01	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	20	0.46	0.01	0.46
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	20	0.46	0.02	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	20	0.46	0.0	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	20	0.46	0.0	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	20	0.46	0.01	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	20	0.46	0.01	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	20	0.46	0.0	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	20	0.46	0.0	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	20	0.46	0.0	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	20	0.46	0.0	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	20	0.46	0.0	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	20	0.46	0.0	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	20	0.46	0.0	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	20	0.46	0.0	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	20	0.46	0.0	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	20	0.46	0.0	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	20	0.45	0.01	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	20	0.45	0.01	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	20	0.45	0.01	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	20	0.45	0.01	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	20	0.45	0.0	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	20	0.45	0.0	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	20	0.45	0.0	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	20	0.45	0.0	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	20	0.45	0.01	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	20	0.45	0.01	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	20	0.45	0.01	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	20	0.45	0.01	0.46
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	20	0.45	0.0	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	20	0.45	0.0	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	20	0.45	0.0	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	20	0.45	0.0	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	20	0.45	0.0	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	20	0.45	0.0	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	20	0.45	0.0	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	20	0.45	0.0	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	20	0.45	0.0	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	20	0.45	0.0	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	20	0.45	0.01	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	20	0.45	0.0	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	20	0.44	0.01	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	20	0.44	0.01	0.44
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	20	0.44	0.14	0.44
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	20	0.44	0.14	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	20	0.44	0.0	0.44
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	20	0.43	0.0	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	20	0.43	0.0	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	20	0.43	0.02	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	20	0.43	0.02	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	20	0.42	0.01	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	20	0.42	0.01	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	20	0.42	0.01	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	20	0.42	0.01	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	20	0.42	0.01	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	20	0.42	0.01	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	20	0.42	0.01	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	20	0.42	0.01	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	20	0.42	0.01	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	20	0.42	0.01	0.42
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	20	0.42	0.01	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	20	0.42	0.01	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	20	0.42	0.01	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	20	0.42	0.01	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	20	0.42	0.0	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	20	0.42	0.0	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	20	0.42	0.0	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	20	0.42	0.0	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	20	0.42	0.0	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	20	0.42	0.0	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	20	0.42	0.0	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	20	0.42	0.0	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	20	0.42	0.0	0.42
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	20	0.42	0.04	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	20	0.42	0.04	0.4
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	20	0.42	0.0	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	20	0.42	0.0	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	20	0.42	0.0	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	20	0.42	0.0	0.42
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	20	0.42	0.05	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	20	0.42	0.05	0.44
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	20	0.42	0.0	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	20	0.42	0.0	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	20	0.42	0.03	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	20	0.42	0.03	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	20	0.42	0.03	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	20	0.42	0.03	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	20	0.42	0.03	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	20	0.42	0.03	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	20	0.41	0.01	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	20	0.41	0.01	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	20	0.41	0.01	0.42
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	20	0.41	0.01	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	20	0.41	0.01	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	20	0.41	0.07	0.42
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	20	0.41	0.01	0.41
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	20	0.41	0.01	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	20	0.41	0.01	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	20	0.41	0.01	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	20	0.41	0.01	0.42
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	20	0.41	0.01	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	20	0.41	0.0	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	20	0.41	0.0	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	20	0.4	0.01	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	20	0.4	0.01	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	20	0.4	0.01	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	20	0.4	0.01	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	20	0.4	0.01	0.41
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	20	0.4	0.0	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	20	0.4	0.0	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	20	0.4	0.0	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	20	0.4	0.05	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	20	0.4	0.05	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	20	0.4	0.05	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	20	0.4	0.05	0.41
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	20	0.4	0.0	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	20	0.4	0.01	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	20	0.4	0.01	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	20	0.4	0.0	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	20	0.4	0.0	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	20	0.4	0.0	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	20	0.39	0.01	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	20	0.39	0.0	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	20	0.39	0.0	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	20	0.39	0.0	0.39
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	20	0.39	0.04	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	20	0.39	0.04	0.37
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	20	0.39	0.0	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	20	0.39	0.0	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	20	0.39	0.0	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	20	0.39	0.01	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	20	0.39	0.0	0.39
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	20	0.39	0.07	0.41
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	20	0.38	0.0	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	20	0.38	0.0	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	20	0.38	0.01	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	20	0.38	0.01	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	20	0.38	0.01	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	20	0.38	0.01	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	20	0.38	0.01	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	20	0.38	0.01	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	20	0.38	0.01	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	20	0.38	0.0	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	20	0.38	0.0	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	20	0.38	0.0	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	20	0.38	0.0	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	20	0.38	0.0	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	20	0.38	0.0	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	20	0.37	0.0	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	20	0.37	0.01	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	20	0.37	0.01	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	20	0.37	0.01	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	20	0.37	0.01	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	20	0.37	0.0	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	20	0.37	0.0	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	20	0.37	0.0	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	20	0.37	0.0	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	20	0.37	0.0	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	20	0.37	0.01	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	20	0.37	0.01	0.37
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	20	0.37	0.02	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	20	0.37	0.02	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	20	0.37	0.02	0.38
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	20	0.37	0.0	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	20	0.37	0.0	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	20	0.37	0.0	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	20	0.37	0.0	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	20	0.37	0.0	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	20	0.37	0.0	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	20	0.37	0.0	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	20	0.37	0.01	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	20	0.37	0.01	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	20	0.37	0.01	0.37
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	20	0.36	0.0	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	20	0.36	0.0	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	20	0.36	0.0	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	20	0.36	0.0	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	20	0.36	0.0	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	20	0.36	0.0	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	20	0.36	0.0	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	20	0.36	0.0	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	20	0.36	0.01	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	20	0.36	0.01	0.36
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	20	0.35	0.0	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	20	0.35	0.0	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	20	0.35	0.0	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	20	0.35	0.0	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	20	0.35	0.01	0.35
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	20	0.35	0.03	0.33
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	20	0.34	0.01	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	20	0.34	0.01	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	20	0.34	0.01	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	20	0.34	0.01	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	20	0.34	0.0	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	20	0.34	0.0	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	20	0.34	0.0	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	20	0.34	0.0	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	20	0.34	0.0	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	20	0.34	0.0	0.34
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	20	0.33	0.0	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	20	0.33	0.0	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	20	0.33	0.01	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	20	0.33	0.0	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	20	0.33	0.0	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	20	0.33	0.01	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	20	0.33	0.01	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	20	0.33	0.01	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	20	0.32	0.01	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	20	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	20	0.32	0.01	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	20	0.32	0.01	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	20	0.32	0.01	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	20	0.32	0.01	0.32
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	20	0.32	0.01	0.32
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	20	0.32	0.01	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	20	0.32	0.01	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	20	0.32	0.01	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	20	0.32	0.01	0.33
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	20	0.32	0.0	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	20	0.32	0.0	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	20	0.32	0.0	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	20	0.32	0.0	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	20	0.32	0.0	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	20	0.32	0.03	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	20	0.32	0.03	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	20	0.32	0.03	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	20	0.32	0.03	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	20	0.32	0.03	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	20	0.32	0.03	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	20	0.31	0.0	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	20	0.31	0.0	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	20	0.31	0.0	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	20	0.31	0.0	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	20	0.31	0.0	0.31
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	20	0.31	0.01	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	20	0.31	0.01	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	20	0.31	0.01	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	20	0.31	0.01	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	20	0.31	0.01	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	20	0.31	0.01	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	20	0.3	0.01	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	20	0.3	0.01	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	20	0.3	0.01	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	20	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	20	0.3	0.01	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	20	0.3	0.01	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	20	0.3	0.01	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	20	0.3	0.0	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	20	0.3	0.0	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	20	0.3	0.0	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	20	0.3	0.0	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	20	0.3	0.0	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	20	0.3	0.0	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	20	0.3	0.0	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	20	0.3	0.0	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	20	0.3	0.0	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	20	0.3	0.0	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	20	0.3	0.01	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	20	0.3	0.01	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	20	0.3	0.0	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	20	0.3	0.0	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	20	0.3	0.01	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	20	0.29	0.01	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	20	0.29	0.0	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	20	0.29	0.0	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	20	0.29	0.0	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	20	0.29	0.0	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	20	0.29	0.0	0.29
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	20	0.29	0.02	0.28
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	20	0.29	0.02	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	20	0.28	0.01	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	20	0.28	0.0	0.28
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	20	0.28	0.04	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	20	0.28	0.04	0.29
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	20	0.27	0.0	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	20	0.27	0.0	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	20	0.27	0.02	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	20	0.27	0.02	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	20	0.27	0.01	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	20	0.27	0.01	0.27
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	20	0.27	0.01	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	20	0.27	0.01	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	20	0.26	0.01	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	20	0.26	0.01	0.26
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	20	0.26	0.06	0.3
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	20	0.26	0.06	0.3
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	20	0.26	0.06	0.3
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	20	0.26	0.06	0.3
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	20	0.26	0.01	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	20	0.26	0.01	0.27
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	20	0.25	0.01	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	20	0.25	0.0	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	20	0.25	0.0	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	20	0.25	0.0	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	20	0.25	0.0	0.25
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	20	0.25	0.03	0.23
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	20	0.25	0.01	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	20	0.25	0.01	0.24
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	20	0.24	0.03	0.24
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.23	0.0	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.23	0.0	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.23	0.0	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	20	0.22	0.01	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	20	0.22	0.0	0.22
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	20	0.22	0.01	0.23
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	20	0.22	0.0	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	20	0.22	0.0	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	20	0.22	0.0	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	20	0.22	0.0	0.22
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	20	0.22	0.04	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	20	0.22	0.04	0.2
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	20	0.22	0.0	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	20	0.22	0.01	0.21
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	20	0.22	0.05	0.21
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	20	0.22	0.05	0.21
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	20	0.21	0.01	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	20	0.21	0.01	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	20	0.21	0.01	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	20	0.21	0.01	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	20	0.21	0.01	0.22
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	20	0.21	0.01	0.2
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	20	0.2	0.02	0.21
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	20	0.2	0.0	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	20	0.2	0.0	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	20	0.2	0.01	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	20	0.2	0.01	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	20	0.2	0.01	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	20	0.2	0.01	0.2
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	20	0.2	0.02	0.19
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	20	0.2	0.02	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	20	0.2	0.01	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	20	0.19	0.03	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	20	0.19	0.03	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	20	0.19	0.03	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	20	0.19	0.03	0.19
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	20	0.19	0.02	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	20	0.19	0.02	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	20	0.19	0.02	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	20	0.18	0.04	0.2
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	20	0.18	0.0	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	20	0.18	0.0	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	20	0.18	0.01	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	20	0.18	0.01	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	20	0.18	0.01	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	20	0.18	0.01	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	20	0.18	0.01	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	20	0.18	0.01	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	20	0.17	0.01	0.18
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	20	0.17	0.0	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	20	0.17	0.0	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	20	0.17	0.0	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	20	0.16	0.01	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	20	0.16	0.01	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	20	0.16	0.01	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	20	0.16	0.01	0.17
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	20	0.16	0.0	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	20	0.16	0.0	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	20	0.16	0.0	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	20	0.16	0.0	0.16
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	20	0.15	0.01	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	20	0.15	0.01	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	20	0.15	0.0	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	20	0.15	0.0	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	20	0.15	0.0	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	20	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	20	0.15	0.0	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	20	0.15	0.0	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	20	0.15	0.01	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	20	0.15	0.01	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	20	0.15	0.01	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	20	0.15	0.01	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	20	0.15	0.04	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	20	0.15	0.01	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	20	0.14	0.01	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	20	0.14	0.01	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	20	0.14	0.01	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	20	0.14	0.01	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	20	0.14	0.0	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	20	0.14	0.0	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	20	0.14	0.0	0.14
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	20	0.14	0.03	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	20	0.13	0.01	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	20	0.13	0.01	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	20	0.13	0.0	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	20	0.13	0.0	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	20	0.13	0.0	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	20	0.13	0.0	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.13	0.0	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.13	0.0	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	20	0.13	0.0	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	20	0.13	0.0	0.13
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	19	0.44	0.07	0.39
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	19	0.44	0.07	0.39
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	19	0.44	0.07	0.39
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	19	0.44	0.07	0.49
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	19	0.33	0.02	0.34
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	19	0.29	0.01	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	19	0.29	0.01	0.3
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	19	0.15	0.01	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	19	0.15	0.01	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	19	0.15	0.01	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	19	0.15	0.01	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	19	0.14	0.0	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	19	0.14	0.0	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	19	0.14	0.0	0.14
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	19	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	19	0.12	0.01	0.12
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	14	0.26	0.01	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	14	0.26	0.01	0.27
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	14	0.17	0.01	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	14	0.17	0.01	0.17
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	13	0.16	0.06	0.14
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	13	0.12	0.01	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	13	0.12	0.01	0.12
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	12	0.21	0.06	0.24
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	12	0.21	0.06	0.24
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	10	0.4	0.0	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	10	0.4	0.0	0.4
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	10	0.26	0.0	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	10	0.26	0.0	0.26
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	10	0.16	0.01	0.16
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	10	0.16	0.01	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	10	0.15	0.04	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	10	0.15	0.04	0.16
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	7	0.24	0.03	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	7	0.24	0.03	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	7	0.24	0.03	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	7	0.24	0.03	0.25
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	6	0.17	0.01	0.17
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	6	0.17	0.01	0.17
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	6	0.16	0.01	0.16
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	6	0.16	0.01	0.16
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	6	0.13	0.03	0.13

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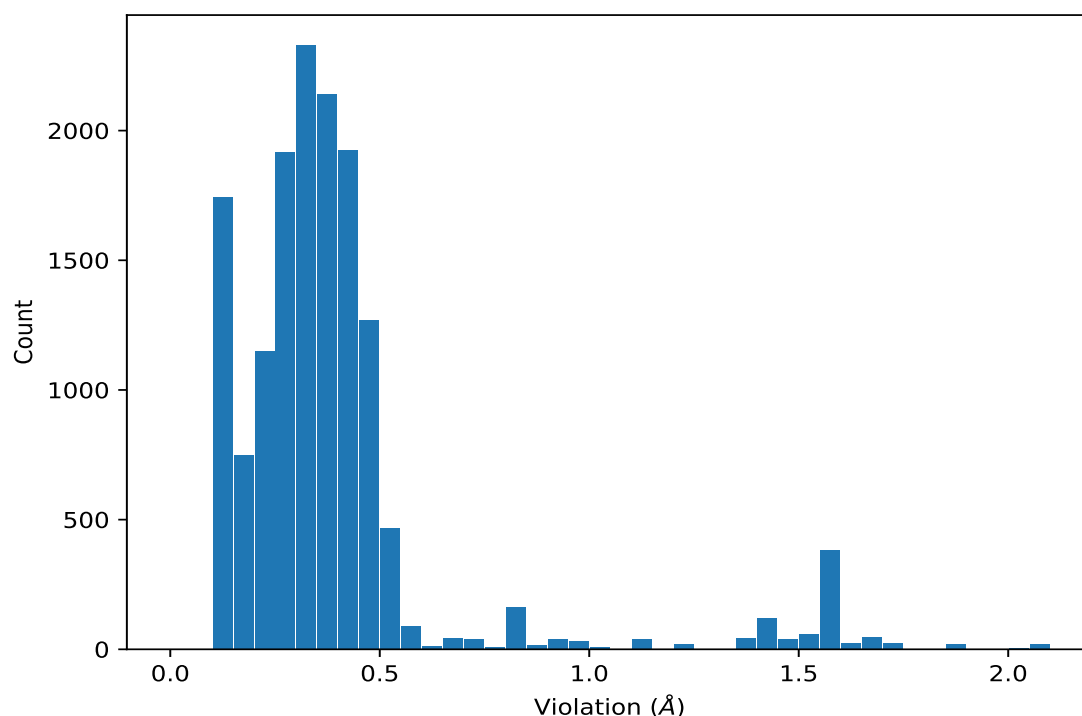
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	6	0.13	0.03	0.13
(2,568)	1:16:A:LYS:HG2	1:16:A:LYS:H	3	0.14	0.0	0.14
(2,568)	1:16:A:LYS:HG3	1:16:A:LYS:H	3	0.14	0.0	0.14
(2,53)	1:3:A:ARG:HB2	1:3:A:ARG:HE	2	0.12	0.0	0.12
(2,53)	1:3:A:ARG:HB3	1:3:A:ARG:HE	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	1	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	1	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	3	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	3	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	4	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	4	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	8	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	8	2.07
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	5	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	5	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	10	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	10	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	13	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	13	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	14	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	14	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	17	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	17	2.06
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	7	2.04
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	7	2.04
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	15	2.02
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	15	2.02
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	18	1.96
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	18	1.96
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	11	1.95
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	11	1.95
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	2	1.9
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	16	1.9
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	1	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	3	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	7	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	9	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	10	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	13	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	14	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	17	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	20	1.89
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	4	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	5	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	6	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	8	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	11	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	12	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	15	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	18	1.88
(1,5)	1:6:A:LYS:O	1:10:A:ASP:H	19	1.88
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	19	1.74
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	19	1.74
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	1	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	2	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	6	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	7	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	9	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	12	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	13	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	16	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	17	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	19	1.73
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	3	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	4	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	5	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	8	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	10	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	11	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	14	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	15	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	18	1.72
(3,3)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.72
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	2	1.7
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	2	1.7
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	16	1.7
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	16	1.7
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	20	1.7
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	20	1.7
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	7	1.69
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	7	1.69
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	1	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	1	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	2	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	2	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	3	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	3	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	4	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	4	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	5	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	5	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	8	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	8	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	9	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	9	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	10	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	10	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	11	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	11	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	12	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	12	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	13	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	13	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	14	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	14	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	15	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	15	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	16	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	16	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	17	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	17	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	18	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	18	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	19	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	19	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	20	1.68
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	20	1.68
(2,254)	1:7:A:PHE:HE1	1:11:A:DPN:HB3	6	1.67
(2,254)	1:7:A:PHE:HE2	1:11:A:DPN:HB3	6	1.67
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	6	1.63
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	6	1.63
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	9	1.61
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	9	1.61
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD2	12	1.61
(2,453)	1:11:A:DPN:HB3	1:16:A:LYS:HD3	12	1.61
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	2	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	2	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	6	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	6	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	7	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	7	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	9	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	9	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	12	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	12	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	15	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	15	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	16	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	16	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	19	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	19	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	20	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	20	1.6
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	3	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	3	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	8	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	8	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	10	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	10	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	11	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	11	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	14	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	14	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	17	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	17	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	18	1.58
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	18	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	6	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	6	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	6	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	9	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	9	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	9	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	12	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	12	1.58
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	12	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	6	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	6	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	6	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	9	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	9	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	9	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	12	1.58
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	12	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	12	1.58
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	2	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	9	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	15	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	16	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	19	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	2	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	2	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	2	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	2	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	2	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	2	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	9	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	15	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	16	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	19	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	20	1.57
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	20	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	1	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	1	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	4	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	4	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	5	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	5	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB2	13	1.57
(2,426)	1:11:A:DPN:HB3	1:13:A:LEU:HB3	13	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	1	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	1	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	1	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	2	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	2	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	2	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	3	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	3	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	3	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	4	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	4	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	4	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	5	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	5	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	5	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	7	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	7	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	7	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	8	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	8	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	8	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	10	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	10	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	10	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	11	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	11	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	11	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	13	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	13	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	13	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	14	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	14	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	14	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	15	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	15	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	15	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	16	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	16	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	16	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	17	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	17	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	17	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	18	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	18	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	18	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	19	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	19	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	19	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	20	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	20	1.57
(2,414)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	1	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	1	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	1	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	2	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	2	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	2	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	3	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	3	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	3	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	4	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	4	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	4	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	5	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	5	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	5	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	7	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	7	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	7	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	8	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	8	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	8	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	10	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	10	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	10	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	11	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	11	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	11	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	13	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	13	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	13	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	14	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	14	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	14	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	15	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	15	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	15	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	16	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	16	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	16	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	17	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	17	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	17	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	18	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	18	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	18	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	19	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	19	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	19	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD11	20	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD12	20	1.57
(2,410)	1:11:A:DPN:HB3	1:12:A:ILE:HD13	20	1.57
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	6	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	7	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	10	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	11	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	12	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	12	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	12	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	12	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	12	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	12	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	18	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	6	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	7	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	10	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	11	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	12	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	18	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	18	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	18	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	18	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	18	1.56
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	18	1.56
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	1	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	3	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	4	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	5	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	8	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	13	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	14	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	14	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	14	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	14	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	14	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	14	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	17	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	17	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	17	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	17	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	17	1.55
(2,428)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	1	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	3	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	4	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	5	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	8	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	13	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	13	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	13	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	13	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	13	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	13	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	14	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD11	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD12	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD13	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD21	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD22	17	1.55
(2,427)	1:11:A:DPN:HB3	1:13:A:LEU:HD23	17	1.55
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	1	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	2	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	3	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	4	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	5	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	6	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	7	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	8	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	9	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	10	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	11	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	12	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	13	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	14	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	15	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	16	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	17	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	18	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	19	1.53
(1,1)	1:4:A:LEU:O	1:8:A:PHE:H	20	1.53
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	5	1.51
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	18	1.51
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	5	1.51
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	18	1.51
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	1	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	2	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	3	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	4	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	6	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	7	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	8	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	9	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	10	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	11	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	12	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	13	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	14	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	15	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	16	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	17	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	19	1.5
(2,300)	1:8:A:PHE:HA	1:11:A:DPN:HB3	20	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	1	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	2	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	3	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	4	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	6	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	7	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	8	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	9	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	10	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	11	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	12	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	13	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	14	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	15	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	16	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	17	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	19	1.5
(2,299)	1:8:A:PHE:HA	1:11:A:DPN:HB3	20	1.5
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	2	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	2	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	5	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	5	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	7	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	7	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	14	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	14	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	15	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	15	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	16	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	16	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	17	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	17	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	19	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	19	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	20	1.47
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	20	1.47
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	1	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	1	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	3	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	3	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	4	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	4	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	6	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	6	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	8	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	8	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	9	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	9	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	10	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	10	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	11	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	11	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	12	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	12	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	13	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	13	1.46
(2,252)	1:7:A:PHE:HD1	1:11:A:DPN:HB3	18	1.46
(2,252)	1:7:A:PHE:HD2	1:11:A:DPN:HB3	18	1.46
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	1	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	1	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	2	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	2	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	3	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	3	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	4	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	4	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	6	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	6	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	7	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	7	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	8	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	8	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	9	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	9	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	10	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	10	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	11	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	11	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	12	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	12	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	13	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	13	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	14	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	14	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	15	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	15	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	16	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	16	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	17	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	17	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	18	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	18	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	19	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	19	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	20	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	20	1.45
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG12	5	1.44
(2,411)	1:11:A:DPN:HB3	1:12:A:ILE:HG13	5	1.44
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	2	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	6	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	9	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	12	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	16	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	19	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	20	1.43
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	2	1.43
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	7	1.43
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	2	1.43
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	7	1.43
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	1	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	3	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	4	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	5	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	7	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	10	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	11	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	13	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	14	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	15	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	17	1.42
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	18	1.42
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	2	1.42
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	7	1.42
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	16	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	1	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	4	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	5	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	6	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	8	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	9	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	10	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	11	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	12	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	13	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	14	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	15	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	16	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	17	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	18	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	19	1.42
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	20	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	1	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	4	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	5	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	6	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	8	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	9	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	10	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	11	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	12	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	13	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	14	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	15	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	16	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	17	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	18	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	19	1.42
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	20	1.42
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	16	1.41
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	16	1.41
(2,409)	1:11:A:DPN:HB3	1:12:A:ILE:HA	8	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	1	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	3	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	4	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	5	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	8	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	10	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	11	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	13	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	14	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	15	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	17	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	18	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	19	1.41
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	20	1.41
(2,351)	1:9:A:ARG:HA	1:11:A:DPN:HB3	3	1.41
(2,350)	1:9:A:ARG:HA	1:11:A:DPN:HB3	3	1.41
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	2	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	2	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	7	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	7	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	12	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	12	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	15	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	15	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	19	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	19	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	20	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	20	1.4
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	6	1.4
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	9	1.4
(2,357)	1:9:A:ARG:H	1:11:A:DPN:HB3	12	1.4
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	6	1.39
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	6	1.39
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	9	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	9	1.39
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	18	1.39
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	18	1.39
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	1	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	1	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	3	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	3	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	4	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	4	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	5	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	5	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	8	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	8	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	10	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	10	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	11	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	11	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	13	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	13	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	14	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	14	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE21	17	1.38
(2,445)	1:11:A:DPN:HB3	1:14:A:GLN:HE22	17	1.38
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	2	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	6	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	9	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	12	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	16	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	19	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	20	1.23
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	1	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	3	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	4	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	5	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	7	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	10	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	11	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	13	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	14	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	15	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	17	1.22
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	18	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,413)	1:11:A:DPN:HB3	1:12:A:ILE:HA	8	1.21
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	1	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	2	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	3	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	5	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	6	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	7	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	8	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	10	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	11	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	12	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	13	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	14	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	15	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	16	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	17	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	18	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	19	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	20	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	1	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	2	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	3	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	5	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	6	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	7	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	8	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	10	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	11	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	12	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	13	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	14	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	15	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	16	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	17	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	18	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	19	1.13
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	20	1.13
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	4	1.12
(2,404)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	9	1.12
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	4	1.12
(2,402)	1:11:A:DPN:HB3	1:11:A:DPN:HZ	9	1.12
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	2	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	3	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	5	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	9	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	10	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	12	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	14	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	15	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	17	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	19	1.0
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	1	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	4	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	6	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	7	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	8	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	11	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	13	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	16	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	18	0.99
(1,2)	1:4:A:LEU:O	1:8:A:PHE:N	20	0.99
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	1	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	2	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	7	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	8	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	10	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	13	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	14	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	15	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	16	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	17	0.96
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	19	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	1	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	2	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	7	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	8	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	10	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	13	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	14	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	15	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	16	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	17	0.96
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	19	0.96
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	2	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	7	0.95
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	15	0.95
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	19	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	3	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	4	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	5	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	6	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	9	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	11	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	12	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	18	0.95
(2,383)	1:10:A:ASP:H	1:11:A:DPN:HB3	20	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	3	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	4	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	5	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	6	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	9	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	11	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	12	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	18	0.95
(2,382)	1:10:A:ASP:H	1:11:A:DPN:HB3	20	0.95
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	1	0.94
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	13	0.94
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	16	0.94
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	17	0.94
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	20	0.94
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	3	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	4	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	5	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	6	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	8	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	9	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	10	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	11	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD12	12	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD11	14	0.93
(3,2)	1:11:A:DPN:HA	1:12:A:ILE:HD13	18	0.93
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	17	0.88
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	2	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	4	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	5	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	13	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	14	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	18	0.87
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	1	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	6	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	7	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	8	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	11	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	12	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	16	0.86
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	20	0.86
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	2	0.85
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	15	0.85
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	15	0.85
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	15	0.85
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	15	0.85
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	15	0.85
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	19	0.85
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	16	0.84
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	19	0.84
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	20	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	3	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	3	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	4	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	4	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	5	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	5	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	8	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	8	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	10	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	10	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	11	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	11	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	13	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	13	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	18	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	18	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	19	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	19	0.84
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	20	0.84
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	20	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	3	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	3	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	4	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	4	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	5	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	5	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	8	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	8	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	10	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	10	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	11	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	11	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	13	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	13	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	18	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	18	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	19	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	19	0.84
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	20	0.84
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	20	0.84
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	6	0.83
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	7	0.83
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	9	0.83
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	12	0.83
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	15	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	1	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	1	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	2	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	2	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	6	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	6	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	7	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	7	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	9	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	9	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	12	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	12	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	14	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	14	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	16	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	16	0.83
(2,378)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	17	0.83
(2,378)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	17	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	1	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	1	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	2	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	2	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	6	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	6	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	7	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	7	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	9	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	9	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	12	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	12	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	14	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	14	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	16	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	16	0.83
(2,374)	1:10:A:ASP:HB2	1:11:A:DPN:HB3	17	0.83
(2,374)	1:10:A:ASP:HB3	1:11:A:DPN:HB3	17	0.83
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	10	0.83
(1,3)	1:5:A:SER:O	1:9:A:ARG:H	3	0.82
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	11	0.81
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	18	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	1	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	2	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	7	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	14	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	16	0.81
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	17	0.81
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	1	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	3	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	4	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	5	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	8	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	10	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	13	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	14	0.8
(2,430)	1:11:A:DPN:HB3	1:13:A:LEU:H	17	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	1	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	2	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	3	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	4	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	6	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	7	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	8	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	9	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	10	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	11	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	12	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	13	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	14	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	15	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	16	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	17	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	18	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	19	0.8
(2,403)	1:11:A:DPN:HB3	1:11:A:DPN:H	20	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	1	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	2	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	3	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	4	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	5	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	6	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	7	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	8	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	9	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	10	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	11	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	12	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	13	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	14	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	15	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	16	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	17	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	18	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	19	0.8
(2,401)	1:11:A:DPN:HB3	1:11:A:DPN:H	20	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	3	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	4	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	5	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	6	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	8	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	9	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	11	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	12	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	13	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	15	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	18	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	19	0.8
(1,6)	1:6:A:LYS:O	1:10:A:ASP:N	20	0.8
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	7	0.76
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	15	0.76
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	2	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	1	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	2	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	7	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	14	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	15	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	16	0.75
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	17	0.75
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	16	0.74
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	19	0.74
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	20	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	3	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	4	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	5	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	8	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	10	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	11	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	13	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	18	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	19	0.74
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	20	0.74
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	6	0.73
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	7	0.73
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	9	0.73
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	12	0.73
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	15	0.73
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	6	0.73
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	9	0.73
(2,371)	1:10:A:ASP:HA	1:11:A:DPN:HB3	12	0.73
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	2	0.72
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	16	0.72
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	20	0.72
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	3	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	4	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	5	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	6	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	8	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	10	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	11	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	12	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	13	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	14	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	17	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	18	0.71
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	19	0.71
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	11	0.71
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	18	0.71
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	9	0.7
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	9	0.7
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	11	0.7
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	18	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	1	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	3	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	4	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	5	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	8	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	10	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	13	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	14	0.7
(2,429)	1:11:A:DPN:HB3	1:13:A:LEU:H	17	0.7
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	2	0.69
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	7	0.69
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	15	0.69
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	16	0.69
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	19	0.69
(3,6)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	20	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	1	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	3	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	4	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	6	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	8	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	10	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	12	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	13	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	14	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	17	0.69
(2,451)	1:11:A:DPN:HB3	1:15:A:ARG:H	5	0.68
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	6	0.68
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	9	0.68
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	12	0.68
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	2	0.67
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	16	0.67
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	20	0.67
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	7	0.66
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	15	0.66
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	19	0.66
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	11	0.65
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	18	0.65
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	1	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	3	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	4	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	5	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	10	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	13	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	14	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	17	0.64
(2,446)	1:11:A:DPN:HB3	1:14:A:GLN:H	8	0.63
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	5	0.61
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	5	0.61
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	5	0.61
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	5	0.61
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	1	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	1	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	4	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	4	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	11	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	11	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	14	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	14	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	17	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	17	0.6
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	2	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	2	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	3	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	3	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	5	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	5	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	6	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	6	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	7	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	7	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	8	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	8	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	9	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	9	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	10	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	10	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	12	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	12	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	13	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	13	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	15	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	15	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	16	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	16	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	18	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	18	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	19	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	19	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE1	20	0.59
(2,301)	1:8:A:PHE:HA	1:11:A:DPN:HE2	20	0.59
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	6	0.58
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	9	0.58
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	12	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	2	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	2	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	3	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	3	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	9	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	9	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	10	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	10	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	12	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	12	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	14	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	14	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	15	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	17	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	17	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	19	0.58
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	19	0.58
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	2	0.57
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	16	0.57
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	20	0.57
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	5	0.57
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	5	0.57
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	7	0.56
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	15	0.56
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	19	0.56
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	5	0.56
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	13	0.56
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	11	0.55
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	18	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	1	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	2	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	3	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	4	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	6	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	7	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	8	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	9	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	10	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	11	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	12	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	14	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	15	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	16	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	17	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	18	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	19	0.55
(2,405)	1:11:A:DPN:H	1:11:A:DPN:HZ	20	0.55
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	1	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	3	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	4	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	5	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	10	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	13	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	14	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	5	0.54
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	5	0.54
(2,444)	1:11:A:DPN:HB3	1:14:A:GLN:H	8	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	1	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	3	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	4	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	5	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	6	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	8	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	9	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	10	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	11	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	12	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	13	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	14	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	17	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	18	0.53
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	5	0.53
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	5	0.53
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	2	0.52
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	7	0.52
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	15	0.52
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	16	0.52
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	19	0.52
(2,303)	1:8:A:PHE:HA	1:11:A:DPN:HZ	20	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	2	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	3	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	4	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	5	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	6	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	7	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	8	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	9	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	10	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	11	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	12	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	13	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	14	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	15	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	16	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	17	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	18	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	19	0.52
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	20	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	1	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	1	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	4	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	4	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	6	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	6	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	8	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	8	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	9	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	9	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	10	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	10	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	11	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	11	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	12	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	12	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	13	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	13	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	14	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	14	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	17	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	17	0.52
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	18	0.52
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	18	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	1	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	1	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	2	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	2	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	4	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	4	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	6	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	6	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	7	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	7	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	8	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	8	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	11	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	11	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	13	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	13	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	14	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	14	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	15	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	15	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	16	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	16	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	18	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	18	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	19	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	19	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	20	0.52
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	20	0.52
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	13	0.52
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	9	0.52
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	9	0.52
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	9	0.52
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	12	0.52
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	12	0.52
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	12	0.52
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	15	0.52
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	15	0.52
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	15	0.52
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	17	0.52
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	17	0.52
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	17	0.52
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	19	0.52
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	19	0.52
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	19	0.52
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	8	0.51
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	9	0.51
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	12	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	3	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	3	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	4	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	4	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	5	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	5	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	6	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	6	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	8	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	8	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	9	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	10	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	10	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	11	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	11	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	12	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	12	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	13	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	13	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	15	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	15	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	18	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	18	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	19	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	19	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	20	0.51
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	20	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	3	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	3	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	4	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	4	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	5	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	5	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	6	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	6	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	8	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	8	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	9	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	9	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	10	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	10	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	11	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	11	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	12	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	12	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	13	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	13	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	15	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	15	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	18	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	18	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	19	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	20	0.51
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	20	0.51
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	4	0.51
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	18	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	1	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	1	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	2	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	2	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	3	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	3	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	4	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	4	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	6	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	6	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	7	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	7	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	8	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	8	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	9	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	9	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	10	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	10	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	11	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	11	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	12	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	12	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	13	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	13	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	14	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	14	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	15	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	15	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	16	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	16	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	17	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	17	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	18	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	18	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	19	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	19	0.51
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	20	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	20	0.51
(2,250)	1:7:A:PHE:H	1:10:A:ASP:HA	1	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	2	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	2	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	3	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	3	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	7	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	7	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	15	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	15	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	16	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	16	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	19	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	19	0.51
(2,233)	1:7:A:PHE:HE1	1:8:A:PHE:H	20	0.51
(2,233)	1:7:A:PHE:HE2	1:8:A:PHE:H	20	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	3	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	3	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	9	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	9	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	10	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	10	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	12	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	12	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	17	0.51
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	17	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	2	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	2	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	2	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	2	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	9	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	9	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	9	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	9	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	12	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	12	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	12	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	12	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	14	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	14	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	14	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	15	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	15	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	15	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	15	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	17	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	17	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	17	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	17	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	19	0.51
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	19	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	19	0.51
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	19	0.51
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	4	0.51
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	8	0.51
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	2	0.51
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	2	0.51
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	2	0.51
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	14	0.51
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	14	0.51
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	14	0.51
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	1	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	2	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	3	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	4	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	5	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	6	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	10	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	11	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	13	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD11	14	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	15	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	16	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	17	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	18	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	19	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD13	20	0.5
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	12	0.5
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	3	0.5
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	3	0.5
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	3	0.5
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	3	0.5
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	3	0.5
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	8	0.5
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	8	0.5
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	8	0.5
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	8	0.5
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	8	0.5
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	8	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	1	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	1	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	2	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	2	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	7	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	7	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	14	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	14	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	16	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	16	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB2	17	0.5
(2,344)	1:9:A:ARG:HA	1:10:A:ASP:HB3	17	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	1	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	1	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	2	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	2	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	7	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	7	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	14	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	14	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	16	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	16	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB2	17	0.5
(2,343)	1:9:A:ARG:HA	1:10:A:ASP:HB3	17	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	1	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	2	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	3	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	5	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	6	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	7	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	8	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	9	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	10	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	11	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	13	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	14	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	15	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	16	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	17	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	19	0.5
(2,297)	1:8:A:PHE:H	1:10:A:ASP:HA	20	0.5
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE1	5	0.5
(2,269)	1:8:A:PHE:HA	1:8:A:PHE:HE2	5	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	1	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	1	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	1	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	1	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	2	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	2	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	2	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	2	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	3	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	3	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	3	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	3	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	4	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	4	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	4	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	4	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	5	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	5	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	5	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	5	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	6	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	6	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	6	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	6	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	7	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	7	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	7	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	7	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	8	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	8	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	8	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	8	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	9	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	9	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	9	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	10	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	10	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	10	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	10	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	11	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	11	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	11	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	11	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	12	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	12	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	12	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	12	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	13	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	13	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	13	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	13	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	14	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	14	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	14	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	14	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	15	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	15	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	15	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	15	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	17	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	17	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	17	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	17	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	18	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	18	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	18	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	18	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	20	0.5
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	20	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	20	0.5
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	20	0.5
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB2	5	0.5
(2,192)	1:5:A:SER:H	1:8:A:PHE:HB3	5	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	1	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	3	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	3	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	4	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	4	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	6	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	6	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	7	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	7	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	8	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	8	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	9	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	9	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	10	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	10	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	11	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	11	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	13	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	13	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	16	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	16	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	17	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	17	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	18	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	18	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	20	0.5
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	20	0.5
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	1	0.5
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	11	0.5
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	16	0.5
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	18	0.5
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	20	0.5
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	3	0.5
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	3	0.5
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	3	0.5
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	10	0.5
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	10	0.5
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	10	0.5
(3,1)	1:10:A:ASP:H	1:12:A:ILE:HD12	7	0.49
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	7	0.49
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	7	0.49
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	15	0.49
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	3	0.49
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	8	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	1	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	1	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	2	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	2	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	3	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	3	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	4	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	4	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	5	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	5	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	6	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	6	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	7	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	7	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	8	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	8	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	9	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	9	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	10	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	10	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	11	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	11	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	12	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	12	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	13	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	13	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	14	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	14	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	15	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	15	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	16	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	16	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	17	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	17	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	18	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	18	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	19	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	19	0.49
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE1	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,384)	1:10:A:ASP:H	1:11:A:DPN:HE2	20	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	1	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	1	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	2	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	2	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	6	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	6	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	9	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	9	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	12	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	12	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	14	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	14	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	16	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	16	0.49
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	17	0.49
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	17	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	1	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	1	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	2	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	2	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	6	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	6	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	9	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	9	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	12	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	12	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	14	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	14	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	16	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	16	0.49
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	17	0.49
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	17	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	1	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	1	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	2	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	2	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	3	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	3	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	4	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	4	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	5	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	6	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	6	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	7	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	7	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	8	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	8	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	9	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	9	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	10	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	10	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	11	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	11	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	12	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	12	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	13	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	13	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	14	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	14	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	15	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	15	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	16	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	16	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	17	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	17	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	18	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	18	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	19	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	19	0.49
(2,296)	1:8:A:PHE:HE1	1:10:A:ASP:H	20	0.49
(2,296)	1:8:A:PHE:HE2	1:10:A:ASP:H	20	0.49
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	16	0.49
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	16	0.49
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	16	0.49
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	16	0.49
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB2	19	0.49
(2,240)	1:7:A:PHE:HE1	1:9:A:ARG:HB3	19	0.49
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB2	19	0.49
(2,240)	1:7:A:PHE:HE2	1:9:A:ARG:HB3	19	0.49
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	7	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	2	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	5	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	5	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	12	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	12	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	14	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	14	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	15	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	15	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE1	19	0.49
(2,178)	1:5:A:SER:H	1:7:A:PHE:HE2	19	0.49
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	3	0.49
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	3	0.49
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	3	0.49
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	3	0.49
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	10	0.49
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	10	0.49
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	10	0.49
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	10	0.49
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	6	0.49
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	7	0.49
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	2	0.48
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	2	0.48
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	16	0.48
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	16	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	1	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	1	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	1	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	1	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	1	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	1	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	4	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	4	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	4	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	4	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	4	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	4	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	5	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	5	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	5	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	5	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	5	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	10	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	10	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	10	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	10	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	10	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	10	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	11	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	11	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	11	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	11	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	11	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	11	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	13	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	13	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	13	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	13	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	13	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	13	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	14	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	14	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	14	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	14	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	14	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	14	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	17	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	17	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	17	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	17	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	17	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	17	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	18	0.48
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	18	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	18	0.48
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	18	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	18	0.48
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	18	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	3	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	3	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	5	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	5	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	8	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	9	0.48
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	9	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	3	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	3	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	4	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	4	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	5	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	5	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	7	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	7	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	8	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	8	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	10	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	10	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	11	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	11	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	13	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	13	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	15	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	15	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	18	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	18	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	19	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	19	0.48
(2,381)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	20	0.48
(2,381)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	20	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	3	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	3	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	4	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	4	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	5	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	5	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	7	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	7	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	8	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	8	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	10	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	10	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	11	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	11	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	13	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	15	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	15	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	18	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	18	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	19	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	19	0.48
(2,377)	1:10:A:ASP:HB2	1:11:A:DPN:HZ	20	0.48
(2,377)	1:10:A:ASP:HB3	1:11:A:DPN:HZ	20	0.48
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	5	0.48
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	5	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	1	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	2	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	3	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	4	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	5	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	6	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	8	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	9	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	10	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	11	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	12	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	13	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	14	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	15	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	16	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	17	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	18	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	19	0.48
(2,234)	1:7:A:PHE:H	1:8:A:PHE:HA	20	0.48
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	5	0.48
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	5	0.48
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	7	0.48
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	7	0.48
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	11	0.48
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	11	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	1	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	4	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	6	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	7	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	8	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	11	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	16	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	18	0.48
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	20	0.48
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	19	0.47
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	19	0.47
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	20	0.47
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	20	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	6	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	6	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	6	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	6	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	6	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	6	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	9	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	9	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	9	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	9	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	9	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	9	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	12	0.47
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	12	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	12	0.47
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	12	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	12	0.47
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	12	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	1	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	1	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	4	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	4	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	6	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	6	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	10	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	10	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	11	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	11	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	12	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	12	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	13	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	13	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	14	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	14	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	17	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	18	0.47
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	18	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	1	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	1	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	3	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	3	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	4	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	4	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	5	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	5	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	8	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	8	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	9	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	9	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	10	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	10	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	11	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	11	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	13	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	13	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	14	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	14	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	17	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	17	0.47
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	18	0.47
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	18	0.47
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	13	0.47
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	13	0.47
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	14	0.47
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	14	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	1	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	1	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	2	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	2	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	3	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	3	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	4	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	4	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	5	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	5	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	6	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	7	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	7	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	8	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	8	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	9	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	9	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	10	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	10	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	11	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	11	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	12	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	12	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	13	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	13	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	14	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	14	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	15	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	15	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	16	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	16	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	17	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	17	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	18	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	18	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	19	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	19	0.47
(2,217)	1:7:A:PHE:HD1	1:7:A:PHE:H	20	0.47
(2,217)	1:7:A:PHE:HD2	1:7:A:PHE:H	20	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	1	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	1	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	2	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	2	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	3	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	3	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	4	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	4	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	6	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	6	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	7	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	7	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	8	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	9	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	9	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	10	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	10	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	11	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	11	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	12	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	12	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	13	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	13	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	14	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	14	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	15	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	15	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	16	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	16	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	17	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	17	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	18	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	18	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	19	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	19	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB2	20	0.47
(2,198)	1:5:A:SER:H	1:9:A:ARG:HB3	20	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	2	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	3	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	10	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	12	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	14	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	15	0.47
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	19	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	2	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	3	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	9	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	10	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	15	0.47
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	17	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	1	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	1	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	4	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	6	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	6	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	8	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	8	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	13	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	13	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	16	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	16	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	18	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	18	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	20	0.47
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	20	0.47
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	1	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	1	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	3	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	3	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	4	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	4	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	5	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	5	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	8	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	8	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	10	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	10	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	11	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	11	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	13	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	13	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	14	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	14	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	17	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	17	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	18	0.46
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	18	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	1	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	1	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	3	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	3	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	4	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	4	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	5	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	8	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	8	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	10	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	10	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	11	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	11	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	13	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	13	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	14	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	14	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	17	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	17	0.46
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	18	0.46
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	18	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	1	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	1	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	3	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	3	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	4	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	4	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	5	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	5	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	6	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	6	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	8	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	8	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	9	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	9	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	10	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	10	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	11	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	11	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	12	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	12	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	13	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	13	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	14	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	14	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	17	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	17	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	18	0.46
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	18	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	1	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	1	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	3	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	3	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	4	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	4	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	5	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	5	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	6	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	6	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	8	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	8	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	9	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	9	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	10	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	10	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	11	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	11	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	12	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	12	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	13	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	13	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	14	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	14	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	17	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	17	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	18	0.46
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	18	0.46
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	5	0.46
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	13	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	2	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	2	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	6	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	6	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	7	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	7	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	12	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	12	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	15	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	15	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	16	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	19	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	19	0.46
(2,416)	1:11:A:DPN:HE1	1:12:A:ILE:HB	20	0.46
(2,416)	1:11:A:DPN:HE2	1:12:A:ILE:HB	20	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	1	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	1	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	3	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	3	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	4	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	4	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	6	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	6	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	8	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	8	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	9	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	9	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	10	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	10	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	11	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	11	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	12	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	12	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	15	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	15	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	17	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	17	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	18	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	18	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	19	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	19	0.46
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	20	0.46
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	20	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	1	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	1	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	1	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	1	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	2	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	2	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	2	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	2	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	3	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	3	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	3	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	4	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	4	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	4	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	4	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	5	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	5	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	5	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	5	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	6	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	6	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	6	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	6	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	7	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	7	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	7	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	7	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	8	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	8	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	8	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	8	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	9	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	9	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	9	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	9	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	10	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	10	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	10	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	10	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	11	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	11	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	11	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	11	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	12	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	12	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	12	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	12	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	13	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	13	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	13	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	14	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	14	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	14	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	14	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	15	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	15	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	15	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	15	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	16	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	16	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	16	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	16	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	17	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	17	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	17	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	17	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	18	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	18	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	18	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	18	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	19	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	19	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	19	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	19	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	20	0.46
(2,276)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	20	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	20	0.46
(2,276)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	20	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	1	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	1	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	1	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	1	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	2	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	2	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	2	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	2	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	3	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	3	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	3	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	3	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	4	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	4	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	4	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	5	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	5	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	5	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	5	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	6	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	6	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	6	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	6	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	7	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	7	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	7	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	7	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	8	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	8	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	8	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	8	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	9	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	9	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	9	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	9	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	10	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	10	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	10	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	10	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	11	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	11	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	11	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	11	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	12	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	12	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	12	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	12	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	13	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	13	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	13	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	13	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	14	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	14	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	14	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	15	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	15	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	15	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	15	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	16	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	16	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	16	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	16	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	17	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	17	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	17	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	17	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	18	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	18	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	18	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	18	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	19	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	19	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	19	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	19	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE1	20	0.46
(2,272)	1:8:A:PHE:HB2	1:8:A:PHE:HE2	20	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE1	20	0.46
(2,272)	1:8:A:PHE:HB3	1:8:A:PHE:HE2	20	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	1	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	1	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	1	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	1	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	3	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	3	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	3	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	3	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	4	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	4	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	4	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	4	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	5	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	5	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	5	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	5	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	10	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	10	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	10	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	11	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	11	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	11	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	11	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	13	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	13	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	13	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	13	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	14	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	14	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	14	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	14	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	17	0.46
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	17	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	17	0.46
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	17	0.46
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	5	0.46
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	5	0.46
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	5	0.46
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	5	0.46
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	14	0.46
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	14	0.46
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	14	0.46
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	14	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	1	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	1	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	2	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	2	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	4	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	4	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	5	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	5	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	6	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	6	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	7	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	7	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	8	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	8	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	9	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	11	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	11	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	13	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	13	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	16	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	16	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	17	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	17	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	18	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	18	0.46
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	20	0.46
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	20	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	1	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	4	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	5	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	6	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	7	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	8	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	9	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	11	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	13	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	16	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	17	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	18	0.46
(2,141)	1:4:A:LEU:HA	1:8:A:PHE:H	20	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	1	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	4	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	5	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	6	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	7	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	8	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	11	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	12	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	13	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	14	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	16	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	18	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	19	0.46
(2,122)	1:4:A:LEU:HA	1:7:A:PHE:H	20	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	2	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	2	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	9	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	12	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	12	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	14	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	14	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	15	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	15	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	17	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	17	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	19	0.46
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	19	0.46
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	3	0.46
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	10	0.46
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	6	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	6	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	7	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	7	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	9	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	9	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	12	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	12	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	15	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	15	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	19	0.45
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	19	0.45
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	6	0.45
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	6	0.45
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	7	0.45
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	7	0.45
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	9	0.45
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	9	0.45
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	12	0.45
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	12	0.45
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	15	0.45
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	15	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	6	0.45
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	6	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	9	0.45
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	9	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	11	0.45
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	11	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	12	0.45
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	18	0.45
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	18	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	2	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	2	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	2	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	2	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	2	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	2	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	7	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	7	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	7	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	7	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	7	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	7	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	15	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	15	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	15	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	15	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	15	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	15	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	16	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	16	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	16	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	16	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	16	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	16	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	19	0.45
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	19	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	19	0.45
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	19	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	19	0.45
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	19	0.45
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	7	0.45
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	7	0.45
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	15	0.45
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	15	0.45
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	7	0.45
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	7	0.45
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	15	0.45
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	15	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	3	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	4	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	7	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	8	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	10	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	11	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	14	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	15	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	17	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	18	0.45
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	19	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	7	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	7	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	15	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	15	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	19	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	19	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	20	0.45
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	20	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	1	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	2	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	5	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	7	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	14	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	15	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	16	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	17	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	18	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	19	0.45
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	20	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	1	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	1	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	2	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	2	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	3	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	3	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	4	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	4	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	5	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	5	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	7	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	10	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	10	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	11	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	11	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	12	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	12	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	13	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	13	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	14	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	14	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	15	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	15	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	16	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	16	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	17	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	17	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	18	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	18	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	19	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	19	0.45
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	20	0.45
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	20	0.45
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	2	0.45
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	2	0.45
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	7	0.45
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	7	0.45
(2,285)	1:8:A:PHE:HE1	1:9:A:ARG:HA	16	0.45
(2,285)	1:8:A:PHE:HE2	1:9:A:ARG:HA	16	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	2	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	2	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	2	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	2	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	6	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	6	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	6	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	6	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	7	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	7	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	7	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	7	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	8	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	8	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	8	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	9	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	9	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	9	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	9	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	12	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	12	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	12	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	12	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	15	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	15	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	15	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	15	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	16	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	16	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	16	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	16	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	18	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	18	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	18	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	18	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	19	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	19	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	19	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	19	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB2	20	0.45
(2,265)	1:7:A:PHE:HE1	1:13:A:LEU:HB3	20	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB2	20	0.45
(2,265)	1:7:A:PHE:HE2	1:13:A:LEU:HB3	20	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	1	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	1	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	1	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	1	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	2	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	2	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	2	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	2	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	3	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	3	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	3	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	4	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	4	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	4	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	4	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	6	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	6	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	6	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	6	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	7	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	7	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	7	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	7	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	8	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	8	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	8	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	8	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	9	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	9	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	9	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	9	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	10	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	10	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	10	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	10	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	11	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	11	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	11	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	11	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	12	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	12	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	12	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	12	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	13	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	13	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	13	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	13	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	15	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	15	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	15	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	15	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	16	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	16	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	16	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	17	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	17	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	17	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	17	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	18	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	18	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	18	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	18	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	19	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	19	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	19	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	19	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB2	20	0.45
(2,222)	1:7:A:PHE:HB2	1:8:A:PHE:HB3	20	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB2	20	0.45
(2,222)	1:7:A:PHE:HB3	1:8:A:PHE:HB3	20	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	3	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	3	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	10	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	10	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	12	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	12	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	14	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	14	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	15	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	15	0.45
(2,218)	1:7:A:PHE:HE1	1:7:A:PHE:H	19	0.45
(2,218)	1:7:A:PHE:HE2	1:7:A:PHE:H	19	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	1	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	1	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	1	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	1	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	2	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	2	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	2	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	2	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	3	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	3	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	3	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	4	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	4	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	4	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	4	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	5	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	5	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	5	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	5	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	6	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	6	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	6	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	6	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	7	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	7	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	7	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	7	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	8	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	8	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	8	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	8	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	9	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	9	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	9	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	9	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	10	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	10	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	10	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	10	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	11	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	11	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	11	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	11	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	12	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	12	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	12	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	12	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	13	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	13	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	13	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	13	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	14	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	14	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	14	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	15	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	15	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	15	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	15	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	16	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	16	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	16	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	16	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	17	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	17	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	17	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	17	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	18	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	18	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	18	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	18	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	19	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	19	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	19	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	19	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	20	0.45
(2,215)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	20	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	20	0.45
(2,215)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	20	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	3	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	3	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	5	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	5	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB2	10	0.45
(2,112)	1:4:A:LEU:HG	1:5:A:SER:HB3	10	0.45
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	9	0.45
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	15	0.45
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	17	0.45
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	19	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	6	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	6	0.45
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	6	0.45
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	6	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	7	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	7	0.45
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	7	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	11	0.45
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	11	0.45
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	11	0.45
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	11	0.45
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	2	0.44
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	2	0.44
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	16	0.44
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	16	0.44
(2,543)	1:14:A:GLN:HG2	1:15:A:ARG:H	20	0.44
(2,543)	1:14:A:GLN:HG3	1:15:A:ARG:H	20	0.44
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	2	0.44
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	2	0.44
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	16	0.44
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	16	0.44
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	19	0.44
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	19	0.44
(2,542)	1:14:A:GLN:HG2	1:15:A:ARG:HA	20	0.44
(2,542)	1:14:A:GLN:HG3	1:15:A:ARG:HA	20	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	1	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	1	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	2	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	2	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	3	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	3	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	4	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	4	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	5	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	5	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	8	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	8	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	10	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	10	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	13	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	13	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	14	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	14	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	16	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	16	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	17	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	19	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	19	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	20	0.44
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	20	0.44
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD2	20	0.44
(2,487)	1:12:A:ILE:HD11	1:15:A:ARG:HD3	20	0.44
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD2	20	0.44
(2,487)	1:12:A:ILE:HD12	1:15:A:ARG:HD3	20	0.44
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD2	20	0.44
(2,487)	1:12:A:ILE:HD13	1:15:A:ARG:HD3	20	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	2	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	2	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	16	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	16	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	19	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	19	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	20	0.44
(2,448)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	20	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	2	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	2	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	16	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	16	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	19	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	19	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB2	20	0.44
(2,447)	1:11:A:DPN:HZ	1:14:A:GLN:HB3	20	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	2	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	6	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	9	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	12	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	16	0.44
(2,439)	1:11:A:DPN:HZ	1:13:A:LEU:H	20	0.44
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	2	0.44
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	2	0.44
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG12	16	0.44
(2,423)	1:11:A:DPN:HZ	1:12:A:ILE:HG13	16	0.44
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	3	0.44
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	3	0.44
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	3	0.44
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	3	0.44
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	8	0.44
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	8	0.44
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	8	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	1	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	1	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	1	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	1	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	7	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	7	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	7	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	7	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	14	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	14	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	14	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	14	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	17	0.44
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	17	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	17	0.44
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	17	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	1	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	1	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	1	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	1	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	7	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	7	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	7	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	7	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	14	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	14	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	14	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	14	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	17	0.44
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	17	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	17	0.44
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	17	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	3	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	4	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	6	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	8	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	9	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	10	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	11	0.44
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,358)	1:9:A:ARG:H	1:11:A:DPN:H	13	0.44
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	6	0.44
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	6	0.44
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	8	0.44
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	8	0.44
(2,356)	1:9:A:ARG:HB2	1:11:A:DPN:H	9	0.44
(2,356)	1:9:A:ARG:HB3	1:11:A:DPN:H	9	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	3	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	4	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	6	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	8	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	9	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	10	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	11	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	12	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	13	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	14	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	15	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	17	0.44
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	18	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	3	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	3	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	5	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	5	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	6	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	6	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	8	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	8	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	9	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	9	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	10	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	10	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	12	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	12	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	14	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	14	0.44
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	18	0.44
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	18	0.44
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	1	0.44
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	1	0.44
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	3	0.44
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	5	0.44
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	5	0.44
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	5	0.44
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	5	0.44
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	2	0.44
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	5	0.44
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	12	0.44
(2,86)	1:3:A:ARG:HA	1:7:A:PHE:H	14	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	1	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	1	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	1	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	1	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	4	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	4	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	4	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	4	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	8	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	8	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	8	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	8	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	13	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	13	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	13	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	13	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	16	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	16	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	16	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	16	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	18	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	18	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	18	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	18	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB2	20	0.44
(2,82)	1:3:A:ARG:HB2	1:5:A:SER:HB3	20	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB2	20	0.44
(2,82)	1:3:A:ARG:HB3	1:5:A:SER:HB3	20	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	1	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	4	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	6	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	7	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	8	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	13	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	16	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	18	0.44
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	20	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	1	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	1	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	4	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	4	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	6	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	6	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	7	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	7	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	8	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	8	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	11	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	11	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	13	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	13	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	16	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	16	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	18	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	18	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	20	0.44
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	20	0.44
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	3	0.44
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	3	0.44
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	3	0.44
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	3	0.44
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	10	0.44
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	10	0.44
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	10	0.44
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	10	0.44
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	7	0.43
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	7	0.43
(2,540)	1:14:A:GLN:HE21	1:15:A:ARG:HA	15	0.43
(2,540)	1:14:A:GLN:HE22	1:15:A:ARG:HA	15	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	1	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	1	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	1	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	1	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	4	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	4	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	4	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	5	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	5	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	5	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	5	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	6	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	6	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	6	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	6	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	9	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	9	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	9	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	9	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	10	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	10	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	10	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	10	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	11	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	11	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	11	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	11	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	12	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	12	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	12	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	12	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	13	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	13	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	13	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	13	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	14	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	14	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	14	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	14	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	17	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	17	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	17	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	17	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	18	0.43
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	18	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	18	0.43
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	2	0.43
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	2	0.43
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	2	0.43
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	2	0.43
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	16	0.43
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	16	0.43
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	16	0.43
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	16	0.43
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	2	0.43
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	2	0.43
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	2	0.43
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	2	0.43
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	16	0.43
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	16	0.43
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	16	0.43
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	16	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	1	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	1	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	1	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	1	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	5	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	5	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	5	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	5	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	10	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	10	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	10	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	10	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	14	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	14	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	14	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	14	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	17	0.43
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	17	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	17	0.43
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	17	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	1	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	2	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	5	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	7	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	16	0.43
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,310)	1:8:A:PHE:H	1:11:A:DPN:HZ	20	0.43
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	12	0.43
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	14	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	2	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	2	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	7	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	7	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	15	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	15	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	16	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	16	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	19	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	19	0.43
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	20	0.43
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	20	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	1	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	1	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	4	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	4	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	11	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	11	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	13	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	13	0.43
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	17	0.43
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	17	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	2	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	2	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	4	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	4	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	6	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	6	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	7	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	7	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	8	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	8	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	9	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	9	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	10	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	10	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	11	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	11	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	12	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	12	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	13	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	13	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	14	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	14	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	15	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	15	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	16	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	16	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	17	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	17	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	18	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	18	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	19	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	19	0.43
(2,255)	1:7:A:PHE:HE1	1:11:A:DPN:H	20	0.43
(2,255)	1:7:A:PHE:HE2	1:11:A:DPN:H	20	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	3	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	3	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	4	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	4	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	5	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	5	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	6	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	6	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	8	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	8	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	9	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	9	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	11	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	11	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	13	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	13	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	18	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	18	0.43
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	20	0.43
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	20	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	2	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	2	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	2	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	2	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	2	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	3	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	5	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	9	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	10	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	15	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	17	0.43
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	19	0.43
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	19	0.43
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	19	0.43
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	19	0.43
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	2	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	3	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	5	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	9	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	10	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	15	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	17	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	17	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	17	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	17	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	17	0.43
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	19	0.43
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	19	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	2	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	2	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	9	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	9	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	12	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	12	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	14	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	14	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	15	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	15	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	19	0.43
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	19	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	1	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	4	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	6	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	7	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	7	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	7	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	7	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	7	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	8	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	11	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	13	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	16	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	18	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	20	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	20	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	20	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	20	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	20	0.43
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	20	0.43
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	3	0.43
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	10	0.43
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	6	0.42
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	11	0.42
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	1	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	1	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	1	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	3	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	3	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	3	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	4	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	4	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	4	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	5	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	5	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	5	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	6	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	6	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	6	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	8	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	8	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	8	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	9	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	9	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	9	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	10	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	10	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	10	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	11	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	11	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	11	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	12	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	12	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	12	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	13	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	13	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	13	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	14	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	14	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	14	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	17	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	17	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	17	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	18	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	18	0.42
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	2	0.42
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	7	0.42
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	15	0.42
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	16	0.42
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	19	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	3	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	3	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	3	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	3	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	4	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	4	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	4	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	4	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	5	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	5	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	5	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	5	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	6	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	6	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	6	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	6	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	8	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	8	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	8	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	8	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	9	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	9	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	9	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	9	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	10	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	10	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	10	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	10	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	11	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	11	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	11	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	11	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	12	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	12	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	12	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	12	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	13	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	13	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	13	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	15	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	15	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	15	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	15	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	18	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	18	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	18	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	18	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	19	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	19	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	19	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	19	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	20	0.42
(2,379)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	20	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	20	0.42
(2,379)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	20	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	3	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	3	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	3	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	3	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	4	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	4	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	4	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	4	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	5	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	5	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	5	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	5	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	6	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	6	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	6	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	6	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	8	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	8	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	8	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	8	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	9	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	9	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	9	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	10	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	10	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	10	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	10	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	11	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	11	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	11	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	11	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	12	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	12	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	12	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	12	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	13	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	13	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	13	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	13	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	15	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	15	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	15	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	15	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	18	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	18	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	18	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	18	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	19	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	19	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	19	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	19	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE1	20	0.42
(2,375)	1:10:A:ASP:HB2	1:11:A:DPN:HE2	20	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE1	20	0.42
(2,375)	1:10:A:ASP:HB3	1:11:A:DPN:HE2	20	0.42
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	1	0.42
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	5	0.42
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	14	0.42
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	17	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	1	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	1	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	2	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	2	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	5	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	7	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	7	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	8	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	8	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	9	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	9	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	10	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	10	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	12	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	12	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	13	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	13	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	14	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	14	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	15	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	15	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	16	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	16	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	17	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	17	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	18	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	18	0.42
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	19	0.42
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	19	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	2	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	2	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	2	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	2	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	3	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	3	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	3	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	3	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	4	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	4	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	4	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	4	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	6	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	6	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	6	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	6	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	7	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	7	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	7	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	8	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	8	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	8	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	8	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	9	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	9	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	9	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	9	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	11	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	11	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	11	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	11	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	12	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	12	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	12	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	12	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	13	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	13	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	13	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	13	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	15	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	15	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	15	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	15	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	16	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	16	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	16	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	16	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	18	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	18	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	18	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	18	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	19	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	19	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	19	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	19	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB2	20	0.42
(2,323)	1:8:A:PHE:HD1	1:13:A:LEU:HB3	20	0.42
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB2	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:8:A:PHE:HD2	1:13:A:LEU:HB3	20	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	1	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	1	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	1	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	1	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	3	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	3	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	3	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	3	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	4	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	4	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	4	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	4	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	5	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	5	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	5	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	5	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	6	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	6	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	6	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	6	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	8	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	8	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	8	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	8	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	9	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	9	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	9	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	9	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	10	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	10	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	10	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	10	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	11	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	11	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	11	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	11	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	12	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	12	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	12	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	12	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	13	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	13	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	13	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	17	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	17	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	17	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	17	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	18	0.42
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	18	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	18	0.42
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	18	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	1	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	2	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	3	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	4	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	5	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	6	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	8	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	9	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	10	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	11	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	13	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	15	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	16	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	17	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	18	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	19	0.42
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	20	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	1	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	1	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	2	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	2	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	3	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	3	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	4	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	4	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	5	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	5	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	6	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	6	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	7	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	9	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	9	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	10	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	10	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	11	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	11	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	12	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	12	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	13	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	13	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	14	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	14	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	15	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	15	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	16	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	16	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	17	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	17	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	19	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	19	0.42
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	20	0.42
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	20	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	1	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	1	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	2	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	2	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	3	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	3	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	4	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	4	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	5	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	5	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	6	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	6	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	7	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	7	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	9	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	9	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	10	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	10	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	11	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	12	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	12	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	13	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	13	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	14	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	14	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	15	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	15	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	16	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	16	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	17	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	17	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	19	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	19	0.42
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	20	0.42
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	20	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	1	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	1	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	3	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	3	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	4	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	4	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	5	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	5	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	6	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	6	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	8	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	8	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	9	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	9	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	10	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	10	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	11	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	11	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	12	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	12	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	13	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	13	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	14	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	14	0.42
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	17	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	17	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,262)	1:7:A:PHE:HE1	1:12:A:ILE:H	18	0.42
(2,262)	1:7:A:PHE:HE2	1:12:A:ILE:H	18	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	1	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	1	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	2	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	2	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	7	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	7	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	10	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	10	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	12	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	12	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	14	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	14	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	15	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	15	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	16	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	16	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	17	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	17	0.42
(2,247)	1:7:A:PHE:HB2	1:10:A:ASP:HA	19	0.42
(2,247)	1:7:A:PHE:HB3	1:10:A:ASP:HA	19	0.42
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	9	0.42
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	9	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	1	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	4	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	6	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	6	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	6	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	6	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	6	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	7	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	8	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	11	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	12	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	13	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	14	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	16	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	16	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	16	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	16	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	16	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	16	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	18	0.42
(2,135)	1:4:A:LEU:HD11	1:7:A:PHE:H	20	0.42
(2,135)	1:4:A:LEU:HD12	1:7:A:PHE:H	20	0.42
(2,135)	1:4:A:LEU:HD13	1:7:A:PHE:H	20	0.42
(2,135)	1:4:A:LEU:HD21	1:7:A:PHE:H	20	0.42
(2,135)	1:4:A:LEU:HD22	1:7:A:PHE:H	20	0.42
(2,135)	1:4:A:LEU:HD23	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	1	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	4	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	6	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	7	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	8	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	8	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	8	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	8	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	8	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	11	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	12	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	13	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	14	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	16	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	18	0.42
(2,129)	1:4:A:LEU:HD11	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD12	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD13	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD21	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD22	1:7:A:PHE:H	20	0.42
(2,129)	1:4:A:LEU:HD23	1:7:A:PHE:H	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	17	0.42
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	17	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	2	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	2	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	2	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	2	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	2	0.42
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	2	0.42
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	12	0.42
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	12	0.42
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	12	0.42
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	12	0.42
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	15	0.42
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	15	0.42
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	15	0.42
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	15	0.42
(2,3)	1:2:A:MET:HA	1:2:A:MET:HG2	5	0.42
(2,3)	1:2:A:MET:HA	1:2:A:MET:HG3	5	0.42
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	1	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	1	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	4	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	4	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	5	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	5	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	6	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	6	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	9	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	9	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	10	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	10	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	11	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	11	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	12	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	12	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	13	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	13	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	14	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	14	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	15	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	15	0.41
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	18	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	20	0.41
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	20	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	1	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	4	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	5	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	9	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	10	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	13	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	14	0.41
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	17	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	2	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	2	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	2	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	2	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	7	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	7	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	7	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	7	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	15	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	15	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	15	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	15	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	16	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	16	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	16	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	16	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	19	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	19	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	19	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	19	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG12	20	0.41
(2,418)	1:11:A:DPN:HE1	1:12:A:ILE:HG13	20	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG12	20	0.41
(2,418)	1:11:A:DPN:HE2	1:12:A:ILE:HG13	20	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	1	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	3	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	4	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	5	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	6	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	8	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	9	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	11	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	12	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	13	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	14	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	17	0.41
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	18	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	1	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	1	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	1	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	1	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	3	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	3	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	3	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	3	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	4	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	4	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	4	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	4	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	5	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	5	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	5	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	5	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	8	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	8	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	8	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	8	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	10	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	10	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	10	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	10	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	11	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	11	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	11	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	11	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	13	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	13	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	13	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	13	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	14	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	14	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	14	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	14	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	17	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	17	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	17	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	17	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	18	0.41
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	18	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	18	0.41
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	18	0.41
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	1	0.41
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	14	0.41
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	17	0.41
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	20	0.41
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	2	0.41
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	2	0.41
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	16	0.41
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	16	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	2	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	3	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	4	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	6	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	7	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	8	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	9	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	10	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	11	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	12	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	13	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	16	0.41
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	18	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	5	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	15	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	15	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	15	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	15	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	15	0.41
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	15	0.41
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	3	0.41
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	4	0.41
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	4	0.41
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	6	0.41
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	6	0.41
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	11	0.41
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	11	0.41
(2,326)	1:8:A:PHE:HE1	1:13:A:LEU:HG	20	0.41
(2,326)	1:8:A:PHE:HE2	1:13:A:LEU:HG	20	0.41
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	14	0.41
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	14	0.41
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	14	0.41
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	14	0.41
(2,292)	1:8:A:PHE:HZ	1:9:A:ARG:HA	7	0.41
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	8	0.41
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	8	0.41
(2,278)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	18	0.41
(2,278)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	18	0.41
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	8	0.41
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	8	0.41
(2,274)	1:8:A:PHE:HB2	1:8:A:PHE:HZ	18	0.41
(2,274)	1:8:A:PHE:HB3	1:8:A:PHE:HZ	18	0.41
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	7	0.41
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	7	0.41
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	15	0.41
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	15	0.41
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	1	0.41
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	1	0.41
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	17	0.41
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	17	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	1	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	1	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	2	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	2	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	3	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	3	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	4	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	4	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	6	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	6	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	7	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	8	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	8	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	10	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	10	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	11	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	11	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	12	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	12	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	13	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	13	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	14	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	14	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	15	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	15	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	16	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	16	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	17	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	17	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	18	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	18	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	19	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	19	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE1	20	0.41
(2,137)	1:4:A:LEU:HG	1:7:A:PHE:HE2	20	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	2	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	2	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	9	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	9	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	12	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	12	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	14	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	14	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	15	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	15	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	17	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	17	0.41
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	19	0.41
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	19	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	2	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	3	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	9	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	12	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	14	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	15	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	17	0.41
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	3	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	9	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	10	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	12	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	14	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	15	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	17	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	17	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	17	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	17	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	17	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	17	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	19	0.41
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	19	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	1	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	1	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	1	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	1	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	2	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	2	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	2	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	2	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	6	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	6	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	6	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	6	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	9	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	9	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	9	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	9	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	11	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	11	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	11	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	11	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	14	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	14	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	14	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	14	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	17	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	17	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	17	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	17	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	18	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	18	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	18	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	19	0.41
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	19	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	19	0.41
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	19	0.41
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	6	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	6	0.4
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	11	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	11	0.4
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	13	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	13	0.4
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	17	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	17	0.4
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	18	0.4
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	18	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	2	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	2	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	3	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	3	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	7	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	7	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	8	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	8	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	16	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	16	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	17	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	17	0.4
(2,556)	1:15:A:ARG:HG2	1:16:A:LYS:HA	19	0.4
(2,556)	1:15:A:ARG:HG3	1:16:A:LYS:HA	19	0.4
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	3	0.4
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	3	0.4
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	8	0.4
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	8	0.4
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	8	0.4
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	8	0.4
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	8	0.4
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	8	0.4
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	8	0.4
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	8	0.4
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	8	0.4
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	8	0.4
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	3	0.4
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	3	0.4
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	8	0.4
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	8	0.4
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	8	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	2	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	7	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	15	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	16	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	19	0.4
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	20	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	2	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	2	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	7	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	7	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	7	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	15	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	15	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	15	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	16	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	16	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	16	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	19	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	19	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	19	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD11	20	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD12	20	0.4
(2,422)	1:11:A:DPN:HZ	1:12:A:ILE:HD13	20	0.4
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	2	0.4
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	20	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	2	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	2	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	2	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	7	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	7	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	7	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	15	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	15	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	15	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	16	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	16	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	16	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	19	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	19	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	19	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	20	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	20	0.4
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	20	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	2	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	4	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	5	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	6	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	9	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	11	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	12	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	13	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	14	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	15	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	16	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	17	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	18	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	19	0.4
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	20	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	6	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	6	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	6	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	6	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	9	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	9	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	9	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	9	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	12	0.4
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	12	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	12	0.4
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	12	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	3	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	4	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	5	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	6	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	8	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	9	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	10	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	11	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	12	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	13	0.4
(2,391)	1:10:A:ASP:HA	1:13:A:LEU:HG	18	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	1	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	1	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	7	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	7	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	12	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	12	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	14	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	15	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	15	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	17	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	17	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	19	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	19	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	20	0.4
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	20	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	3	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	3	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	3	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	4	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	4	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	4	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	5	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	5	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	5	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	6	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	6	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	6	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	8	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	8	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	8	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	10	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	10	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	10	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	11	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	11	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	11	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	12	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	12	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	12	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	15	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	15	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	15	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	19	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	19	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	19	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	20	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	20	0.4
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	20	0.4
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	19	0.4
(2,347)	1:9:A:ARG:H	1:10:A:ASP:HA	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	1	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	2	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	3	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	4	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	6	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	7	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	8	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	8	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	8	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	8	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	8	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	9	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	10	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	11	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	12	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	13	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	14	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	16	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	16	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	16	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	16	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	16	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	17	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	18	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	19	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD11	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD12	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD13	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD21	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD22	20	0.4
(2,328)	1:8:A:PHE:HZ	1:13:A:LEU:HD23	20	0.4
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	2	0.4
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	2	0.4
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	16	0.4
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	16	0.4
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	19	0.4
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	19	0.4
(2,259)	1:7:A:PHE:HE1	1:12:A:ILE:HA	20	0.4
(2,259)	1:7:A:PHE:HE2	1:12:A:ILE:HA	20	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	3	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	4	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	6	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	8	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	9	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	10	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	11	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	13	0.4
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	18	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	2	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	2	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	3	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	3	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	4	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	4	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	5	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	5	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	6	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	6	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	7	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	7	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	8	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	8	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	9	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	9	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	10	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	10	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	11	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	11	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	12	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	12	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	13	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	13	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	14	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	14	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	15	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	15	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	16	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	16	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	18	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	18	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	19	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	19	0.4
(2,249)	1:7:A:PHE:HE1	1:10:A:ASP:H	20	0.4
(2,249)	1:7:A:PHE:HE2	1:10:A:ASP:H	20	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	1	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	1	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	4	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	6	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	6	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	7	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	7	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	8	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	8	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	11	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	11	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	13	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	13	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	16	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	16	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	18	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	18	0.4
(2,60)	1:3:A:ARG:HD2	1:3:A:ARG:H	20	0.4
(2,60)	1:3:A:ARG:HD3	1:3:A:ARG:H	20	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	4	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	4	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	4	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	4	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	7	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	7	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	7	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	7	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	8	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	8	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	8	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	8	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	13	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	13	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	13	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	13	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	16	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	16	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	16	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	16	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	20	0.4
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	20	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	20	0.4
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	20	0.4
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	1	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	3	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	3	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	4	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	4	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	5	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	5	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	8	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	8	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	9	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	9	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	10	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	10	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	12	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	12	0.39
(2,571)	1:16:A:LYS:HB2	1:17:A:LYS:H	14	0.39
(2,571)	1:16:A:LYS:HB3	1:17:A:LYS:H	14	0.39
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	2	0.39
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	7	0.39
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	15	0.39
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	16	0.39
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	19	0.39
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	19	0.39
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	19	0.39
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	19	0.39
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	19	0.39
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	12	0.39
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	12	0.39
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	12	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	3	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	6	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	8	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	9	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	10	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	11	0.39
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	18	0.39
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	7	0.39
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	15	0.39
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	16	0.39
(2,408)	1:11:A:DPN:HA	1:12:A:ILE:H	19	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	1	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	1	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	1	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	3	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	3	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	3	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	4	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	4	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	4	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	5	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	5	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	5	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	6	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	6	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	6	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	8	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	8	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	8	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	9	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	9	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	9	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	10	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	10	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	11	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	11	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	11	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	12	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	12	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	12	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	13	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	13	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	13	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	14	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	14	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	14	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	17	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	17	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	17	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD11	18	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD12	18	0.39
(2,406)	1:11:A:DPN:HA	1:12:A:ILE:HD13	18	0.39
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	1	0.39
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	3	0.39
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	8	0.39
(2,400)	1:11:A:DPN:HA	1:11:A:DPN:HZ	10	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	2	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	2	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	2	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	2	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	7	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	7	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	7	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	7	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	16	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	16	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	16	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	16	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	19	0.39
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	19	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	19	0.39
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	2	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	2	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	2	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	2	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	2	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	7	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	15	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	16	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	19	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	20	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	20	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	20	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	20	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	20	0.39
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	2	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	7	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	7	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	7	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	7	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	7	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	15	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	16	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	19	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	20	0.39
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	20	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	3	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	3	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	4	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	4	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	5	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	5	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	6	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	6	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	8	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	8	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	9	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	9	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	10	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	10	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	11	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	13	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	13	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB2	18	0.39
(2,388)	1:10:A:ASP:HA	1:13:A:LEU:HB3	18	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	1	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	1	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	1	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	2	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	2	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	2	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	7	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	7	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	7	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	9	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	9	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	9	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	13	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	13	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	13	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	14	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	14	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	14	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	16	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	16	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	16	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	17	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	17	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	17	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD11	18	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD12	18	0.39
(2,360)	1:9:A:ARG:H	1:12:A:ILE:HD13	18	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	1	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	2	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	4	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	5	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	7	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	9	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	10	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	11	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	12	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	13	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	15	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	16	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	17	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	18	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	19	0.39
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	20	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	1	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	1	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	1	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	2	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	2	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	2	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	3	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	3	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	3	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	4	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	4	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	4	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	5	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	5	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	5	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	6	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	6	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	6	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	7	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	7	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	7	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	8	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	8	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	8	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	9	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	9	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	9	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	10	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	10	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	10	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	11	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	11	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	11	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	12	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	12	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	13	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	13	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	13	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	14	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	14	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	14	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	15	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	15	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	15	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	16	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	16	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	16	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	17	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	17	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	17	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	18	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	18	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	18	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	19	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	19	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	19	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD11	20	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD12	20	0.39
(2,321)	1:8:A:PHE:HZ	1:12:A:ILE:HD13	20	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	2	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	2	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	2	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	2	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	7	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	7	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	7	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	7	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	15	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	15	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	15	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	15	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	16	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	16	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	16	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	16	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	20	0.39
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	20	0.39
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	20	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	1	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	2	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	5	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	7	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	14	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	15	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	16	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	17	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	19	0.39
(2,256)	1:7:A:PHE:H	1:11:A:DPN:HZ	20	0.39
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	7	0.39
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	7	0.39
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	7	0.39
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	5	0.38
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	5	0.38
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	6	0.38
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	6	0.38
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	9	0.38
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	9	0.38
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	12	0.38
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	12	0.38
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	20	0.38
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	20	0.38
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	20	0.38
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	20	0.38
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	20	0.38
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	20	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	1	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	1	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	4	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	4	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	4	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	4	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	4	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	4	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	5	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	5	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	6	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	6	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	9	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	9	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	9	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	9	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	9	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	9	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	10	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	10	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	11	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	11	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	12	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	12	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	13	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	13	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	13	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	13	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	13	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	13	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	14	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	14	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	17	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	17	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	18	0.38
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	18	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	18	0.38
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	18	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	18	0.38
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	18	0.38
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	18	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	18	0.38
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	18	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	18	0.38
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	1	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	1	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	4	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	4	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	5	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	5	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	6	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	6	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	6	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	6	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	6	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	6	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	9	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	9	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	10	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	10	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	11	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	11	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	11	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	11	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	11	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	11	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	12	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	12	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	13	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	13	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	14	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	14	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	17	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	17	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	17	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	17	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	17	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	17	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	18	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	18	0.38
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	18	0.38
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	16	0.38
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	16	0.38
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	16	0.38
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	20	0.38
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	20	0.38
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	20	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	1	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	4	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	5	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	12	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	13	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	14	0.38
(2,460)	1:12:A:ILE:HB	1:12:A:ILE:H	17	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	2	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	2	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	7	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	7	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	15	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	16	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	16	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	19	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	19	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	20	0.38
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	20	0.38
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	15	0.38
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	15	0.38
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	15	0.38
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	15	0.38
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE21	20	0.38
(2,396)	1:10:A:ASP:HB2	1:14:A:GLN:HE22	20	0.38
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE21	20	0.38
(2,396)	1:10:A:ASP:HB3	1:14:A:GLN:HE22	20	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	1	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	5	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	14	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	17	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	17	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	17	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	17	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	17	0.38
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	1	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	1	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	1	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	1	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	1	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	5	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	14	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	17	0.38
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	17	0.38
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	3	0.38
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	6	0.38
(2,352)	1:9:A:ARG:HA	1:11:A:DPN:H	8	0.38
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG12	19	0.38
(2,318)	1:8:A:PHE:HE1	1:12:A:ILE:HG13	19	0.38
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG12	19	0.38
(2,318)	1:8:A:PHE:HE2	1:12:A:ILE:HG13	19	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	1	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	1	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	1	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	1	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	1	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	1	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	3	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	3	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	3	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	3	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	3	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	3	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	4	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	4	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	4	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	4	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	4	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	5	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	5	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	5	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	5	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	5	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	5	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	6	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	6	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	6	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	6	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	6	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	6	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	8	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	8	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	8	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	8	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	8	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	8	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	9	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	9	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	9	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	9	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	9	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	9	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	10	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	10	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	10	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	10	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	10	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	10	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	11	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	11	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	11	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	11	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	11	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	11	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	12	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	12	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	12	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	12	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	12	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	15	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	15	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	15	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	15	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	15	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	15	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	17	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	17	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	17	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	17	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	17	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	17	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	18	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	18	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	18	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	18	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	18	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	18	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	20	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	20	0.38
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	20	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	20	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	20	0.38
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	20	0.38
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	5	0.38
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	5	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	7	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	15	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	16	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	18	0.38
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	19	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	1	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	1	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	3	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	3	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	7	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	7	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	10	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	16	0.38
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	16	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	1	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	1	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	2	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	2	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	3	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	3	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	4	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	4	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	5	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	5	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	6	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	6	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	7	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	7	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	8	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	8	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	9	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	9	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	10	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	10	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	11	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	11	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	12	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	12	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	13	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	13	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	14	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	14	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	15	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	15	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	16	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	16	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	17	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	17	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	18	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	18	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	19	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	19	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB2	20	0.38
(2,235)	1:7:A:PHE:H	1:8:A:PHE:HB3	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	3	0.38
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	17	0.38
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	5	0.38
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	5	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	1	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	1	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	1	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	6	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	6	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	6	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	8	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	8	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	8	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	11	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	11	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	11	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	16	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	16	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	16	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	18	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	18	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	18	0.38
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	20	0.38
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	20	0.38
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	20	0.38
(2,1)	1:2:A:MET:HA	1:2:A:MET:HE1	5	0.38
(2,1)	1:2:A:MET:HA	1:2:A:MET:HE2	5	0.38
(2,1)	1:2:A:MET:HA	1:2:A:MET:HE3	5	0.38
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	1	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	1	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	3	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	3	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	4	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	4	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	8	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	8	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	10	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	10	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	11	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	11	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	13	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	14	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	14	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	17	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	17	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	18	0.37
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	18	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	2	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	2	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	3	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	3	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	4	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	4	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	4	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	4	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	4	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	4	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	7	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	7	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	8	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	8	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	10	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	10	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	11	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	11	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	11	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	11	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	11	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	11	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	14	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	14	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	15	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	15	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	16	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	16	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	16	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	16	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	16	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	16	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	17	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	17	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	19	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	19	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	20	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	20	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	20	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	20	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	20	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	20	0.37
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	2	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	2	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	2	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	2	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	2	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	2	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	3	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	3	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	4	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	4	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	7	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	7	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	7	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	7	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	7	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	7	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	8	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	8	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	10	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	10	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	11	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	11	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	14	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	14	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	14	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	14	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	14	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	14	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	15	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	15	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	16	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	16	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	17	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	17	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	17	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	17	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	17	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	17	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	19	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	19	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	20	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	20	0.37
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	20	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	2	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	2	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	2	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	3	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	3	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	3	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	4	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	4	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	4	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	5	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	5	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	5	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	6	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	6	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	6	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	8	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	8	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	9	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	9	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	9	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	10	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	10	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	10	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	14	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	14	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	14	0.37
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	19	0.37
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	19	0.37
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	19	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	1	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	1	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	3	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	3	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	4	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	4	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	5	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	5	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	6	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	6	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	8	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	8	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	10	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	10	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	11	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	11	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	12	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	12	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	13	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	13	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	14	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	14	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	17	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	17	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	18	0.37
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	3	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	3	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	3	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	3	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	3	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	4	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	6	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	8	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	9	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	10	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	11	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	12	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	12	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	12	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	12	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	12	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	13	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD11	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD12	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD13	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD21	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD22	18	0.37
(2,390)	1:10:A:ASP:HA	1:13:A:LEU:HD23	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	3	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	4	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	6	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	8	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	9	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	9	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	9	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	9	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	9	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	10	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	11	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	12	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	13	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD11	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD12	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD13	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD21	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD22	18	0.37
(2,389)	1:10:A:ASP:HA	1:13:A:LEU:HD23	18	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	2	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	2	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	2	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	2	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	2	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	2	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	7	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	7	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	7	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	7	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	7	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	13	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	13	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	13	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	13	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	13	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	13	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	14	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	14	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	14	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	14	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	14	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	14	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	16	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	16	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	16	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	16	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	16	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	16	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD11	19	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD12	19	0.37
(2,317)	1:8:A:PHE:HE1	1:12:A:ILE:HD13	19	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD11	19	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD12	19	0.37
(2,317)	1:8:A:PHE:HE2	1:12:A:ILE:HD13	19	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	1	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	1	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	2	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	2	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	4	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	4	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	5	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	5	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	7	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	7	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	8	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	8	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	10	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	10	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	11	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	13	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	13	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	14	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	14	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	15	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	15	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	16	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	16	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	18	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	18	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	19	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	19	0.37
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	20	0.37
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	20	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	1	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	1	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	2	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	2	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	3	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	3	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	4	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	4	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	6	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	6	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	7	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	7	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	8	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	8	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	9	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	9	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	10	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	10	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	11	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	11	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	12	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	12	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	13	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	13	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	14	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	14	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	15	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	16	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	16	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	17	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	17	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	18	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	18	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	19	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	19	0.37
(2,267)	1:7:A:PHE:HE1	1:13:A:LEU:HG	20	0.37
(2,267)	1:7:A:PHE:HE2	1:13:A:LEU:HG	20	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	1	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	2	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	3	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	4	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	5	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	6	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	8	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	9	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	10	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	11	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	12	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	13	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	14	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	17	0.37
(2,251)	1:7:A:PHE:H	1:10:A:ASP:H	20	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	2	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	2	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	4	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	4	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	6	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	6	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	8	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	8	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	9	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	9	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	11	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	11	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	12	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	12	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	13	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	13	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	14	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	15	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	15	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	17	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	17	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	18	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	18	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	19	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	19	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	20	0.37
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	20	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	1	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	1	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	2	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	2	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	3	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	3	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	4	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	4	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	6	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	6	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	7	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	7	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	8	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	8	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	9	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	9	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	10	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	10	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	11	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	11	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	12	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	12	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	13	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	13	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	14	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	14	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	15	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	15	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	16	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	16	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	17	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	18	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	18	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	19	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	19	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	20	0.37
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	20	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	2	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	2	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	4	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	4	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	5	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	5	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	9	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	9	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	12	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	12	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	13	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	13	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	14	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	14	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	15	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	15	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	16	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	16	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	17	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	17	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	18	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	18	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	19	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	19	0.37
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	20	0.37
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	20	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	2	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	2	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	4	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	4	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	5	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	5	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	9	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	9	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	12	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	13	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	13	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	14	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	14	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	15	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	15	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	16	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	16	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	17	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	17	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	18	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	18	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	19	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	19	0.37
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	20	0.37
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	20	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	1	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	2	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	4	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	6	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	7	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	8	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	9	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	10	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	11	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	12	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	13	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	14	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	15	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	16	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	18	0.37
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	19	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	1	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	1	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	3	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	3	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	4	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	4	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	6	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	6	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	7	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	8	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	8	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	10	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	10	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	11	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	11	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	16	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	16	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	18	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	18	0.37
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	20	0.37
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	20	0.37
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD11	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD12	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD13	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD21	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD22	5	0.37
(2,23)	1:2:A:MET:HE1	1:4:A:LEU:HD23	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD11	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD12	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD13	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD21	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD22	5	0.37
(2,23)	1:2:A:MET:HE2	1:4:A:LEU:HD23	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD11	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD12	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD13	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD21	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD22	5	0.37
(2,23)	1:2:A:MET:HE3	1:4:A:LEU:HD23	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD11	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD12	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD13	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD21	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD22	5	0.37
(2,22)	1:2:A:MET:HE1	1:4:A:LEU:HD23	5	0.37
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD11	5	0.37
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD12	5	0.37
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD13	5	0.37
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD21	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD22	5	0.37
(2,22)	1:2:A:MET:HE2	1:4:A:LEU:HD23	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD11	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD12	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD13	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD21	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD22	5	0.37
(2,22)	1:2:A:MET:HE3	1:4:A:LEU:HD23	5	0.37
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	4	0.37
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	4	0.37
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	4	0.37
(2,11)	1:2:A:MET:HE1	1:3:A:ARG:HA	13	0.37
(2,11)	1:2:A:MET:HE2	1:3:A:ARG:HA	13	0.37
(2,11)	1:2:A:MET:HE3	1:3:A:ARG:HA	13	0.37
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	2	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	2	0.36
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	7	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	7	0.36
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	15	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	15	0.36
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	16	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	16	0.36
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	19	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	19	0.36
(2,541)	1:14:A:GLN:HE21	1:15:A:ARG:H	20	0.36
(2,541)	1:14:A:GLN:HE22	1:15:A:ARG:H	20	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	1	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	1	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	5	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	5	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	5	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	5	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	5	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	5	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	6	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	6	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	9	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	9	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	12	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	12	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	12	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	12	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	12	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	12	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	13	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	13	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	18	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	18	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	18	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	18	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	18	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	18	0.36
(2,513)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	1	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	1	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	5	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	5	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	5	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	5	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	5	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	5	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	6	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	6	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	9	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	9	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	12	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	12	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	12	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	12	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	12	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	12	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	13	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	13	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD11	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD12	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD13	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD21	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD22	1:14:A:GLN:HG3	18	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG2	18	0.36
(2,510)	1:13:A:LEU:HD23	1:14:A:GLN:HG3	18	0.36
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	1	0.36
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	1	0.36
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	1	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	1	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	1	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	1	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	3	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	3	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	3	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	4	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	4	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	4	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	5	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	5	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	5	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	6	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	6	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	8	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	8	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	8	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	9	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	9	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	9	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	10	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	10	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	10	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	11	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	11	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	11	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	12	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	12	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	12	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	13	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	13	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	13	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	14	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	14	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	14	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	17	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	17	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	17	0.36
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	18	0.36
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	18	0.36
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	18	0.36
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB2	9	0.36
(2,436)	1:11:A:DPN:HZ	1:13:A:LEU:HB3	9	0.36
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	6	0.36
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	9	0.36
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	12	0.36
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	6	0.36
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	9	0.36
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	12	0.36
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	3	0.36
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	3	0.36
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	6	0.36
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	6	0.36
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	9	0.36
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	12	0.36
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	12	0.36
(2,309)	1:8:A:PHE:HE1	1:11:A:DPN:H	17	0.36
(2,309)	1:8:A:PHE:HE2	1:11:A:DPN:H	17	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	1	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	2	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	3	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	4	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	5	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	6	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	7	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	8	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	9	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	10	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	11	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	12	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	13	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	14	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	15	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	16	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	17	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	18	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	19	0.36
(2,271)	1:8:A:PHE:HA	1:8:A:PHE:HZ	20	0.36
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB2	5	0.36
(2,242)	1:7:A:PHE:H	1:9:A:ARG:HB3	5	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	1	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	1	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	2	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	2	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	4	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	4	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	5	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	5	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	7	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	7	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	11	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	11	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	13	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	13	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	16	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	18	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	18	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	20	0.36
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	20	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	1	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	1	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	2	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	2	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	3	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	3	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	4	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	4	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	6	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	6	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	7	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	7	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	8	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	8	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	9	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	9	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	10	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	10	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	11	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	11	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	13	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	13	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	15	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	15	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	16	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	16	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	18	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	18	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	19	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	19	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	20	0.36
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	20	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	1	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	1	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	3	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	3	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	6	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	7	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	7	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	8	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	8	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	10	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	10	0.36
(2,175)	1:5:A:SER:HB2	1:7:A:PHE:H	11	0.36
(2,175)	1:5:A:SER:HB3	1:7:A:PHE:H	11	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	1	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	1	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	3	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	3	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	6	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	6	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	7	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	7	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	8	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	8	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	10	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	10	0.36
(2,173)	1:5:A:SER:HB2	1:7:A:PHE:H	11	0.36
(2,173)	1:5:A:SER:HB3	1:7:A:PHE:H	11	0.36
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	5	0.36
(2,164)	1:4:A:LEU:HA	1:9:A:ARG:H	20	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	1	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	1	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	2	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	2	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	3	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	3	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	4	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	4	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	6	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	6	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	7	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	7	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	8	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	8	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	9	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	9	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	10	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	11	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	11	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	12	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	12	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	13	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	13	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	14	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	14	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	15	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	15	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	16	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	16	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	17	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	17	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	18	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	18	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	19	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	19	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD1	20	0.36
(2,136)	1:4:A:LEU:HG	1:7:A:PHE:HD2	20	0.36
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	5	0.36
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	5	0.36
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	5	0.36
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	5	0.36
(2,84)	1:3:A:ARG:HB2	1:5:A:SER:H	13	0.36
(2,84)	1:3:A:ARG:HB3	1:5:A:SER:H	13	0.36
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	3	0.36
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	3	0.36
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	10	0.36
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	10	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	2	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	4	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	5	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	9	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	17	0.36
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	18	0.36
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	7	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	7	0.35
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	7	0.35
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	11	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	11	0.35
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	13	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	13	0.35
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	13	0.35
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	15	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	15	0.35
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	15	0.35
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	17	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	17	0.35
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	17	0.35
(2,489)	1:12:A:ILE:HD11	1:17:A:LYS:H	18	0.35
(2,489)	1:12:A:ILE:HD12	1:17:A:LYS:H	18	0.35
(2,489)	1:12:A:ILE:HD13	1:17:A:LYS:H	18	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	2	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	2	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	2	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	7	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	7	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	7	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	15	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	15	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	15	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	16	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	16	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	16	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	19	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	19	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	19	0.35
(2,483)	1:12:A:ILE:HD11	1:14:A:GLN:H	20	0.35
(2,483)	1:12:A:ILE:HD12	1:14:A:GLN:H	20	0.35
(2,483)	1:12:A:ILE:HD13	1:14:A:GLN:H	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	1	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	2	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	2	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	2	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	2	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	2	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	3	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	4	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	5	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	6	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	7	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	8	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	9	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	9	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	9	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	9	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	9	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	10	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	11	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	12	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	13	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	14	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	15	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	16	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	16	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	16	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	16	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	16	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	17	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	18	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	19	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD11	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD12	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD13	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD21	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD22	20	0.35
(2,467)	1:12:A:ILE:HA	1:13:A:LEU:HD23	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	1	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	2	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	3	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	3	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	3	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	3	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	3	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	4	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	5	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	6	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	7	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	8	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	9	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	10	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	10	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	10	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	10	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	10	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	11	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	12	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	13	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	14	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	15	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	16	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	17	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	17	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	17	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	17	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	17	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	18	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	19	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD11	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD12	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD13	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD21	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD22	20	0.35
(2,466)	1:12:A:ILE:HA	1:13:A:LEU:HD23	20	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	1	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	3	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	4	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	5	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	10	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	11	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	13	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	14	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	17	0.35
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	18	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	1	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	3	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	4	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	5	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	10	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	11	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	13	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	14	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	17	0.35
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	18	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	1	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	1	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	2	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	3	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	3	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	4	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	4	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	5	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	5	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	6	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	6	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	7	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	7	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	8	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	8	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	9	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	9	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	10	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	10	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	11	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	11	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	12	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	12	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	13	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	13	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	14	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	14	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	15	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	15	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	16	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	16	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	17	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	17	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	18	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	18	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	19	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	19	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB2	20	0.35
(2,281)	1:8:A:PHE:HA	1:9:A:ARG:HB3	20	0.35
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE1	5	0.35
(2,236)	1:7:A:PHE:H	1:8:A:PHE:HE2	5	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	3	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	3	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	6	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	8	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	8	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	9	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	9	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	10	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	10	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	12	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	12	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	14	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	14	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	15	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	15	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	17	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	17	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB2	19	0.35
(2,179)	1:5:A:SER:HA	1:8:A:PHE:HB3	19	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	5	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	5	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	12	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	12	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	14	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	14	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD1	17	0.35
(2,177)	1:5:A:SER:H	1:7:A:PHE:HD2	17	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	2	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	2	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	3	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	3	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	9	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	9	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	10	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	10	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	14	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	14	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	15	0.35
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	15	0.35
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	2	0.35
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	17	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	6	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	8	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	12	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	13	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	14	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	15	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	19	0.35
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	20	0.35
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	2	0.34
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	7	0.34
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	15	0.34
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	16	0.34
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	19	0.34
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	6	0.34
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	9	0.34
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	12	0.34
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	12	0.34
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	12	0.34
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	12	0.34
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	12	0.34
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	12	0.34
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	6	0.34
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	9	0.34
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	12	0.34
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	12	0.34
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	12	0.34
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	12	0.34
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	12	0.34
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	20	0.34
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	20	0.34
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	20	0.34
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	20	0.34
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	20	0.34
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	20	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	2	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	2	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	16	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	16	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	19	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	19	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	19	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	19	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	19	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	19	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	20	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	20	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	20	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	20	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	20	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	20	0.34
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	20	0.34
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	6	0.34
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	9	0.34
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	12	0.34
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	20	0.34
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	20	0.34
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	20	0.34
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	20	0.34
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	20	0.34
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	20	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	2	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	2	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	2	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	2	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	2	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	2	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	16	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	16	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	19	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	19	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	20	0.34
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	20	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	20	0.34
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	20	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	20	0.34
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	20	0.34
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	20	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	20	0.34
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	20	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	20	0.34
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	20	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	1	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	2	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	3	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	4	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	5	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	6	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	7	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	7	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	7	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	7	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	7	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	8	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	9	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	10	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	11	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	12	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	13	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	14	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	14	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	14	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	14	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	14	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	15	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	16	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	17	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	18	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	19	0.34
(2,514)	1:13:A:LEU:HD11	1:14:A:GLN:H	20	0.34
(2,514)	1:13:A:LEU:HD12	1:14:A:GLN:H	20	0.34
(2,514)	1:13:A:LEU:HD13	1:14:A:GLN:H	20	0.34
(2,514)	1:13:A:LEU:HD21	1:14:A:GLN:H	20	0.34
(2,514)	1:13:A:LEU:HD22	1:14:A:GLN:H	20	0.34
(2,514)	1:13:A:LEU:HD23	1:14:A:GLN:H	20	0.34
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	8	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	15	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	15	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	19	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	19	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	20	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	20	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	20	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	20	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	20	0.34
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	20	0.34
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	15	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	15	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	15	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	15	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	15	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	15	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	19	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	19	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	20	0.34
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	20	0.34
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	20	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	2	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	2	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	2	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	16	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	16	0.34
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	16	0.34
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	1	0.34
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	17	0.34
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	4	0.34
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	6	0.34
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	18	0.34
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	5	0.34
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	5	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	1	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	1	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	4	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	4	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	6	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	6	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	7	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	7	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	8	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	8	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	11	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	11	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	12	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	12	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	13	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	13	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	16	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	16	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	17	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	17	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	18	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	18	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	19	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	19	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	20	0.34
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	20	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	1	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	4	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	6	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	7	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	8	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	11	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	13	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	16	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	18	0.34
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	20	0.34
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	9	0.34
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	12	0.34
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	15	0.34
(2,15)	1:2:A:MET:HA	1:4:A:LEU:H	19	0.34
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	1	0.34
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	7	0.34
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	16	0.34
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	3	0.33
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	3	0.33
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	8	0.33
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	8	0.33
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	9	0.33
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	9	0.33
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	12	0.33
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	12	0.33
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	9	0.33
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	12	0.33
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	20	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	1	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	4	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	5	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	10	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	11	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	11	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	11	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	11	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	11	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	13	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	14	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	17	0.33
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	18	0.33
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	18	0.33
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	18	0.33
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	18	0.33
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	18	0.33
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	18	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	1	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	2	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	4	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	4	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	4	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	4	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	4	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	5	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	8	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	10	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	11	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	13	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	14	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	16	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	16	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	16	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	16	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	16	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	17	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	18	0.33
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	19	0.33
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	19	0.33
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	19	0.33
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	19	0.33
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	19	0.33
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	19	0.33
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	7	0.33
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	7	0.33
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	15	0.33
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	15	0.33
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	15	0.33
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	15	0.33
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	15	0.33
(2,519)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	15	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	1	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	2	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	4	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	5	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	8	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	10	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	11	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	11	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	11	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	11	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	11	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	13	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	14	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	16	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	17	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	18	0.33
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	19	0.33
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	19	0.33
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	19	0.33
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	19	0.33
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	19	0.33
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	19	0.33
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	7	0.33
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	7	0.33
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	7	0.33
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	7	0.33
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	7	0.33
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	7	0.33
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD11	1:15:A:ARG:HD3	15	0.33
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD12	1:15:A:ARG:HD3	15	0.33
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD13	1:15:A:ARG:HD3	15	0.33
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD21	1:15:A:ARG:HD3	15	0.33
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD22	1:15:A:ARG:HD3	15	0.33
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD2	15	0.33
(2,517)	1:13:A:LEU:HD23	1:15:A:ARG:HD3	15	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	1	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	1	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	3	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	3	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	4	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	4	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	5	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	5	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	6	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	6	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	8	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	8	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	9	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	9	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	10	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	10	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	12	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	12	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	14	0.33
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	2	0.33
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	16	0.33
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	19	0.33
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	20	0.33
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	2	0.33
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	16	0.33
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	19	0.33
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	20	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	2	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	2	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	7	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	7	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	11	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	11	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	11	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	11	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	11	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	11	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	13	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	13	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	16	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	16	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	16	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	16	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	16	0.33
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	16	0.33
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	2	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	2	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	7	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	7	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	7	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	7	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	7	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	7	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	11	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	11	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	13	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	13	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	16	0.33
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	16	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	16	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	16	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	16	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	16	0.33
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	16	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	1	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	1	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	1	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	3	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	3	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	3	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	4	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	4	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	4	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	6	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	6	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	6	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	7	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	7	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	7	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	10	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	10	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	10	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	11	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	11	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	11	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	14	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	14	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	14	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	15	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	15	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	15	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	19	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	19	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	19	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	20	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	20	0.33
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	20	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	2	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	3	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	4	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	6	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	7	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	8	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	10	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	11	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	12	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	13	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	14	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	15	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	16	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	18	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	19	0.33
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	20	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	1	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	2	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	3	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	5	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	7	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	8	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	9	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	10	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	12	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	13	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	14	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	15	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	16	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	17	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	19	0.33
(2,199)	1:5:A:SER:H	1:9:A:ARG:H	20	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	1	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	1	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	3	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	3	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	4	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	4	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	6	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	6	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	7	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	7	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	8	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	8	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	9	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	9	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	10	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	11	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	11	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	12	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	12	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	13	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	13	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	15	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	15	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	16	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	16	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	17	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	17	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	18	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	18	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	19	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	19	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	20	0.33
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	20	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	1	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	1	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	1	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	1	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	4	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	4	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	4	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	4	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	6	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	6	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	6	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	6	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	7	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	7	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	7	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	7	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	8	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	8	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	8	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	8	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	11	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	11	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	11	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	13	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	13	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	13	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	13	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	16	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	16	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	16	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	16	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	18	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	18	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	18	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	18	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	20	0.33
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	20	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	20	0.33
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	1	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	4	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	6	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	7	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	8	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	8	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	8	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	8	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	8	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	11	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	13	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	16	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	18	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	20	0.33
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	20	0.33
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	6	0.32
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	6	0.32
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	6	0.32
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	11	0.32
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	3	0.32
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	3	0.32
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	3	0.32
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	3	0.32
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	3	0.32
(2,523)	1:13:A:LEU:HD11	1:16:A:LYS:HA	8	0.32
(2,523)	1:13:A:LEU:HD12	1:16:A:LYS:HA	8	0.32
(2,523)	1:13:A:LEU:HD13	1:16:A:LYS:HA	8	0.32
(2,523)	1:13:A:LEU:HD21	1:16:A:LYS:HA	8	0.32
(2,523)	1:13:A:LEU:HD22	1:16:A:LYS:HA	8	0.32
(2,523)	1:13:A:LEU:HD23	1:16:A:LYS:HA	8	0.32
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	3	0.32
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	7	0.32
(2,520)	1:13:A:LEU:HD11	1:15:A:ARG:H	15	0.32
(2,520)	1:13:A:LEU:HD12	1:15:A:ARG:H	15	0.32
(2,520)	1:13:A:LEU:HD13	1:15:A:ARG:H	15	0.32
(2,520)	1:13:A:LEU:HD21	1:15:A:ARG:H	15	0.32
(2,520)	1:13:A:LEU:HD22	1:15:A:ARG:H	15	0.32
(2,520)	1:13:A:LEU:HD23	1:15:A:ARG:H	15	0.32
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	3	0.32
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	7	0.32
(2,518)	1:13:A:LEU:HD11	1:15:A:ARG:H	15	0.32
(2,518)	1:13:A:LEU:HD12	1:15:A:ARG:H	15	0.32
(2,518)	1:13:A:LEU:HD13	1:15:A:ARG:H	15	0.32
(2,518)	1:13:A:LEU:HD21	1:15:A:ARG:H	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	1:13:A:LEU:HD22	1:15:A:ARG:H	15	0.32
(2,518)	1:13:A:LEU:HD23	1:15:A:ARG:H	15	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	11	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	11	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	13	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	13	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	17	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	17	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	18	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	18	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	19	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	19	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	20	0.32
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	20	0.32
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	7	0.32
(2,415)	1:11:A:DPN:HB3	1:12:A:ILE:H	15	0.32
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	7	0.32
(2,412)	1:11:A:DPN:HB3	1:12:A:ILE:H	15	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	3	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	3	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	4	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	4	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	4	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	4	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	4	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	4	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	5	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	5	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	6	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	6	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	8	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	8	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	9	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	9	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	9	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	9	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	9	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	9	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	10	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	10	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	12	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	12	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	18	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	18	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	18	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	18	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	18	0.32
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	18	0.32
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	3	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	3	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	4	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	4	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	5	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	5	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	6	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	6	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	6	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	6	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	6	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	6	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	8	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	8	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	9	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	9	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	10	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	10	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	10	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	10	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	10	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	10	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	12	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	12	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	18	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	18	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	18	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	18	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	18	0.32
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	18	0.32
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	18	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	1	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	1	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	1	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	1	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	2	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	2	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	2	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	2	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	3	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	3	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	3	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	3	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	4	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	4	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	4	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	4	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	5	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	5	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	5	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	6	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	6	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	6	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	6	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	7	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	7	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	7	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	7	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	8	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	8	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	8	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	8	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	9	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	9	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	9	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	9	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	10	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	10	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	10	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	10	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	11	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	11	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	11	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	11	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	12	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	12	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	12	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	12	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	13	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	13	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	13	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	13	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	14	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	14	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	14	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	14	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	15	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	15	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	15	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	16	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	16	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	16	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	16	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	17	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	17	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	17	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	17	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	18	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	18	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	18	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	18	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	19	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	19	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	19	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	19	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE1	20	0.32
(2,354)	1:9:A:ARG:HB2	1:11:A:DPN:HE2	20	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE1	20	0.32
(2,354)	1:9:A:ARG:HB3	1:11:A:DPN:HE2	20	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	5	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	5	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	5	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	8	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	8	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	8	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	9	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	9	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	9	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	12	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	12	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	12	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	13	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	13	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	13	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	17	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	17	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	17	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD11	18	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD12	18	0.32
(2,320)	1:8:A:PHE:H	1:12:A:ILE:HD13	18	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	2	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	2	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	2	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	2	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	2	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	7	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	7	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	7	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	7	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	7	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	7	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	15	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	15	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	15	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	15	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	15	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	15	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	16	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	16	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	16	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	16	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	16	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	16	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	19	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	19	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	19	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	19	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	19	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	19	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	20	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	20	0.32
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	20	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	20	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	20	0.32
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	20	0.32
(2,241)	1:7:A:PHE:H	1:9:A:ARG:HA	5	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	1	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	2	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	3	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	4	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	5	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	7	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	8	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	9	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	10	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	11	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	12	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	13	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	14	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	15	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	16	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	17	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	18	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	19	0.32
(2,220)	1:7:A:PHE:HA	1:8:A:PHE:H	20	0.32
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	2	0.32
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	2	0.32
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE1	14	0.32
(2,140)	1:4:A:LEU:HA	1:8:A:PHE:HE2	14	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	2	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	2	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	3	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	3	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	9	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	9	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	10	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	10	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	12	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	12	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	14	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	14	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	15	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	15	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	19	0.32
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	19	0.32
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	5	0.32
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	5	0.32
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	5	0.32
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	5	0.32
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	2	0.32
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	9	0.32
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	14	0.32
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	2	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	2	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	2	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	2	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	2	0.32
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	2	0.32
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	10	0.32
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	1	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	1	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	3	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	3	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	4	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	4	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	5	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	5	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	8	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	8	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	13	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	13	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	17	0.31
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	17	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	1	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	1	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	3	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	3	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	4	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	4	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	5	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	5	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	8	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	8	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	13	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	13	0.31
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	17	0.31
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	17	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	1	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	3	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	4	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	5	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	8	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	10	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	14	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	17	0.31
(2,525)	1:13:A:LEU:HG	1:16:A:LYS:H	18	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	1	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	1	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	1	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	1	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	1	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	1	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	3	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	3	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	3	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	3	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	3	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	3	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	4	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	4	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	4	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	4	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	4	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	4	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	5	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	5	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	5	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	5	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	5	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	5	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	6	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	6	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	6	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	6	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	6	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	6	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	8	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	8	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	8	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	8	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	8	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	8	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	9	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	9	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	9	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	9	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	9	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	10	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	10	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	10	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	10	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	10	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	10	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	11	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	11	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	11	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	11	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	11	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	11	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	12	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	12	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	12	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	12	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	12	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	12	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	13	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	13	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	13	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	13	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	13	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	13	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	14	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	14	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	14	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	14	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	14	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	14	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	17	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	17	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	17	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	17	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	17	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	17	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	18	0.31
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	18	0.31
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	18	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	18	0.31
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	18	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	2	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	2	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	7	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	7	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	15	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	15	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG2	16	0.31
(2,452)	1:11:A:DPN:HZ	1:15:A:ARG:HG3	16	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	2	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	2	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	16	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	16	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	19	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	19	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	20	0.31
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	20	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	2	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	6	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	7	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	9	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	12	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	15	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	16	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	19	0.31
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	20	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	1	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	1	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	2	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	2	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	3	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	3	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	4	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	4	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	5	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	5	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	7	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	7	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	8	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	10	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	10	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	11	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	11	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	13	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	13	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	14	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	14	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	15	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	15	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	16	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	16	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	17	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	17	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	19	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	19	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	20	0.31
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	20	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	1	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	1	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	14	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	14	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	14	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	14	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	14	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	14	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	17	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	17	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	17	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	17	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	17	0.31
(2,394)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	17	0.31
(2,394)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	1	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	1	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	14	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	14	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD11	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD12	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD13	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD21	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD22	17	0.31
(2,393)	1:10:A:ASP:HB2	1:13:A:LEU:HD23	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD11	17	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD12	17	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD13	17	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD21	17	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD22	17	0.31
(2,393)	1:10:A:ASP:HB3	1:13:A:LEU:HD23	17	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	3	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	3	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	7	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	7	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	11	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	11	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	12	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	12	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	15	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	15	0.31
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	19	0.31
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	19	0.31
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	3	0.31
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	5	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	1	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	1	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	4	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	4	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	5	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	5	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	6	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	6	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	7	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	7	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	8	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	8	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	11	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	11	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	13	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	13	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	16	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	16	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	17	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	17	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	18	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB2	20	0.31
(2,139)	1:4:A:LEU:HA	1:8:A:PHE:HB3	20	0.31
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE1	5	0.31
(2,121)	1:4:A:LEU:HA	1:7:A:PHE:HE2	5	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	2	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	9	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	10	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	12	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	14	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	15	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	17	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	17	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	17	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	17	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	17	0.31
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	19	0.31
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	19	0.31
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	19	0.31
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	19	0.31
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	19	0.31
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	19	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	2	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	2	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	2	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	2	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	12	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	12	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	12	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	12	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	14	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	14	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	14	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	14	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	15	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	15	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	15	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	15	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	17	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	17	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	17	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	17	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	19	0.31
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	19	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	19	0.31
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	19	0.31
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	12	0.31
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	17	0.31
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	19	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	3	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	3	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	3	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	3	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	3	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	9	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	10	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	12	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	14	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	15	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	17	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	19	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	19	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	19	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	19	0.31
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	19	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD11	5	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD12	5	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD13	5	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD21	5	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD22	5	0.31
(2,64)	1:3:A:ARG:HA	1:4:A:LEU:HD23	5	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	4	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	4	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	8	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	8	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	13	0.31
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	13	0.31
(1,4)	1:5:A:SER:O	1:9:A:ARG:N	3	0.31
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	10	0.3
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	10	0.3
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	11	0.3
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	11	0.3
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	14	0.3
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	14	0.3
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	18	0.3
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	18	0.3
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	10	0.3
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	10	0.3
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	11	0.3
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	11	0.3
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	14	0.3
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	14	0.3
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	18	0.3
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	18	0.3
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	18	0.3
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	18	0.3
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	20	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	2	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	2	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	2	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	2	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	2	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	2	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	7	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	7	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	7	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	7	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	7	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	15	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	15	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	15	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	15	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	15	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	15	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	16	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	16	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	16	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	16	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	16	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	16	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	19	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	19	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	19	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	19	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	19	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	19	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG2	20	0.3
(2,482)	1:12:A:ILE:HD11	1:14:A:GLN:HG3	20	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG2	20	0.3
(2,482)	1:12:A:ILE:HD12	1:14:A:GLN:HG3	20	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG2	20	0.3
(2,482)	1:12:A:ILE:HD13	1:14:A:GLN:HG3	20	0.3
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	2	0.3
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	19	0.3
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	20	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	7	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	7	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	12	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	12	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	15	0.3
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	15	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	3	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	8	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	10	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	11	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	17	0.3
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	1	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	2	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	3	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	4	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	5	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	7	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	8	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	10	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	11	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	13	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	14	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	15	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	16	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	17	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	18	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	19	0.3
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	20	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	6	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	6	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	9	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	9	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	12	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	12	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG12	18	0.3
(2,407)	1:11:A:DPN:HA	1:12:A:ILE:HG13	18	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	1	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	1	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	2	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	2	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	3	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	3	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	4	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	4	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	5	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	5	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	6	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	6	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	7	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	7	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	8	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	8	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	9	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	10	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	10	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	11	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	11	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	12	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	12	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	13	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	13	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	14	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	14	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	15	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	15	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	16	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	16	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	17	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	17	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	18	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	18	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	19	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	19	0.3
(2,305)	1:8:A:PHE:HB2	1:11:A:DPN:H	20	0.3
(2,305)	1:8:A:PHE:HB3	1:11:A:DPN:H	20	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	1	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	2	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	3	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	4	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	6	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	7	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	9	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	10	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	12	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	14	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	16	0.3
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	17	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	5	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	5	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	5	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	5	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	5	0.3
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	5	0.3
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	5	0.3
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	5	0.3
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	5	0.3
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	5	0.3
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	5	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	1	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	1	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	1	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	1	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	1	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	1	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	3	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	3	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	3	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	3	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	3	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	3	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	4	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	4	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	4	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	4	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	4	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	4	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	5	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	5	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	5	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	5	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	5	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	5	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	6	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	6	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	6	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	6	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	6	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	6	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	8	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	8	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	8	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	8	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	8	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	8	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	9	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	9	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	9	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	9	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	9	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	10	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	10	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	10	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	10	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	10	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	10	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	11	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	11	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	11	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	11	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	11	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	11	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	12	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	12	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	12	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	12	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	12	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	12	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	13	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	13	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	13	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	13	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	13	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	13	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	14	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	14	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	14	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	14	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	14	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	14	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	17	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	17	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	17	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	17	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	17	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	17	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD11	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD12	18	0.3
(2,260)	1:7:A:PHE:HE1	1:12:A:ILE:HD13	18	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD11	18	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD12	18	0.3
(2,260)	1:7:A:PHE:HE2	1:12:A:ILE:HD13	18	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	1	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	1	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	6	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	6	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	8	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	8	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	10	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	10	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	14	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	14	0.3
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	16	0.3
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	16	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	1	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	7	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	10	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	11	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	12	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	15	0.3
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	19	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	1	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	1	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	1	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	1	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	2	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	2	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	2	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	2	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	3	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	3	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	3	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	3	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	4	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	4	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	4	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	4	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	5	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	5	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	5	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	6	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	6	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	6	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	6	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	7	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	7	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	7	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	7	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	8	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	8	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	8	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	8	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	9	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	9	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	9	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	9	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	10	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	10	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	10	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	10	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	11	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	11	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	11	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	11	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	12	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	12	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	12	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	12	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	13	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	13	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	13	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	13	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	14	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	14	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	14	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	14	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	15	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	15	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	15	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	16	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	16	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	16	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	16	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	17	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	17	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	17	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	17	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	18	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	18	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	18	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	18	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	19	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	19	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	19	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	19	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB2	20	0.3
(2,188)	1:5:A:SER:HB2	1:8:A:PHE:HB3	20	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB2	20	0.3
(2,188)	1:5:A:SER:HB3	1:8:A:PHE:HB3	20	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	1	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	1	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	1	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	1	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	2	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	2	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	2	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	2	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	3	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	3	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	3	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	3	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	4	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	4	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	4	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	4	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	5	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	5	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	5	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	5	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	6	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	6	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	6	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	7	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	7	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	7	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	7	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	8	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	8	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	8	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	8	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	9	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	9	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	9	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	9	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	10	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	10	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	10	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	10	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	11	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	11	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	11	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	11	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	12	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	12	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	12	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	12	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	13	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	13	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	13	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	13	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	14	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	14	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	14	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	14	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	15	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	15	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	15	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	15	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	16	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	16	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	16	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	17	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	17	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	17	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	17	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	18	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	18	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	18	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	18	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	19	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	19	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	19	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	19	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB2	20	0.3
(2,184)	1:5:A:SER:HB2	1:8:A:PHE:HB3	20	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB2	20	0.3
(2,184)	1:5:A:SER:HB3	1:8:A:PHE:HB3	20	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	1	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	4	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	7	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	8	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	11	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	13	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	16	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	18	0.3
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	20	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	1	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	3	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	4	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	4	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	4	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	4	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	4	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	6	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	7	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	8	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	11	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	13	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	16	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	18	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	18	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	18	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	18	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	18	0.3
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	20	0.3
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	20	0.3
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	20	0.3
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	20	0.3
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	20	0.3
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	20	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	3	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	3	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	3	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	3	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	9	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	9	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	9	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	9	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD1	10	0.3
(2,87)	1:3:A:ARG:HB2	1:7:A:PHE:HD2	10	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD1	10	0.3
(2,87)	1:3:A:ARG:HB3	1:7:A:PHE:HD2	10	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	1	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	1	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	1	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	1	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	1	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	1	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	4	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	4	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	4	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	4	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	4	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	4	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	6	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	6	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	6	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	6	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	6	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	6	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	7	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	7	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	7	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	7	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	7	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	8	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	8	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	8	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	8	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	8	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	8	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	11	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	11	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	11	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	11	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	11	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	11	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	13	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	13	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	13	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	13	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	13	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	13	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	16	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	16	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	16	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	16	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	16	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	16	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	18	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	18	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	18	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	18	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	18	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	18	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	20	0.3
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	20	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	20	0.3
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	20	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	20	0.3
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	20	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	1	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	1	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	1	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	1	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	1	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	4	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	4	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	4	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	4	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	4	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	4	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	6	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	6	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	6	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	6	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	6	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	6	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	7	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	7	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	7	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	7	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	7	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	7	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	8	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	8	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	8	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	8	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	8	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	8	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	11	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	11	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	11	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	11	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	11	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	11	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	13	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	13	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	13	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	13	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	13	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	13	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	16	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	16	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	16	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	16	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	16	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	18	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	18	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	18	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	18	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	18	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	18	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	20	0.3
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	20	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	20	0.3
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	20	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	20	0.3
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	20	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	1	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	1	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	6	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	6	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	7	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	7	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	11	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	11	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	16	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	16	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	18	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	18	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB2	20	0.3
(2,6)	1:2:A:MET:HA	1:3:A:ARG:HB3	20	0.3
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	7	0.29
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	7	0.29
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	15	0.29
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	15	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	1	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	1	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	4	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	4	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	5	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	5	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	10	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	10	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	11	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	11	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	13	0.29
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	14	0.29
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	14	0.29
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	2	0.29
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	7	0.29
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	15	0.29
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	16	0.29
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	19	0.29
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	19	0.29
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	19	0.29
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	19	0.29
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	19	0.29
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	19	0.29
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	2	0.29
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	7	0.29
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	15	0.29
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	16	0.29
(2,490)	1:12:A:ILE:H	1:17:A:LYS:HA	19	0.29
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	3	0.29
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	8	0.29
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	7	0.29
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	16	0.29
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	6	0.29
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	6	0.29
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	9	0.29
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	9	0.29
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	1	0.29
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	4	0.29
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	5	0.29
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	13	0.29
(2,425)	1:11:A:DPN:HA	1:13:A:LEU:H	14	0.29
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	6	0.29
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	9	0.29
(2,424)	1:11:A:DPN:HZ	1:12:A:ILE:H	12	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	1	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	1	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	2	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	2	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	3	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	3	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	4	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	4	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	6	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	6	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	7	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	7	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	8	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	8	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	9	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	9	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	10	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	10	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	11	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	11	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	12	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	12	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	13	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	13	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	15	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	15	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	16	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	16	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	17	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	18	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	18	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	19	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	19	0.29
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	20	0.29
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	20	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	5	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	8	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	11	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	13	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	15	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	18	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	19	0.29
(2,289)	1:8:A:PHE:H	1:9:A:ARG:HA	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	1	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	1	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	2	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	2	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	3	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	3	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	3	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	3	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	3	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	3	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	4	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	4	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	6	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	6	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	7	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	7	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	7	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	7	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	7	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	7	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	8	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	8	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	9	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	9	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	10	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	10	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	11	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	11	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	11	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	11	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	11	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	11	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	12	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	12	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	13	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	13	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	14	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	14	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	14	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	14	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	14	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	14	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	15	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	15	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	17	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	17	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	18	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	18	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	19	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	19	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	19	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	19	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	19	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	19	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	20	0.29
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	20	0.29
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	20	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	2	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	2	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	4	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	4	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	5	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	5	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	9	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	9	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	13	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	13	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	18	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	18	0.29
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	20	0.29
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	20	0.29
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	6	0.29
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	8	0.29
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	14	0.29
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	16	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	1	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	1	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	1	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	1	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	1	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	2	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	3	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	4	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	6	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	7	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	8	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	9	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	9	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	9	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	9	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	9	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	10	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	11	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	12	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	14	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	15	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	16	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	17	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	17	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	17	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	17	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	17	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	18	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	19	0.29
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	20	0.29
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	20	0.29
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	20	0.29
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	20	0.29
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	20	0.29
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	20	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	1	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	2	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	3	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	4	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	4	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	4	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	4	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	4	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	6	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	7	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	8	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	9	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	10	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	11	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	12	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	12	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	12	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	12	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	12	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	14	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	15	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	16	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	17	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	18	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	19	0.29
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	20	0.29
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	20	0.29
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	20	0.29
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	20	0.29
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	20	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	2	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	3	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	6	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	9	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	10	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	12	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	14	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	15	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	17	0.29
(2,142)	1:4:A:LEU:HA	1:8:A:PHE:HZ	19	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	2	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	2	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	9	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	9	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	12	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	12	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	14	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	14	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	15	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	15	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	17	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	17	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	19	0.29
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	19	0.29
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	3	0.29
(2,77)	1:3:A:ARG:H	1:4:A:LEU:HA	10	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	3	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	3	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	3	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	3	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	3	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	3	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	9	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	9	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	9	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	9	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	9	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	9	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	10	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	10	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	10	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	10	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	10	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	12	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	12	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	12	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	12	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	12	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	12	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	14	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	14	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	14	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	14	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	14	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	14	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	15	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	15	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	15	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	15	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	15	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	15	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	17	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	17	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	17	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	17	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	17	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	17	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	19	0.29
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	19	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	19	0.29
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	19	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	19	0.29
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	19	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	3	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	3	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	3	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	3	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	3	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	3	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	9	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	9	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	9	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	9	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	9	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	10	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	10	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	10	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	10	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	10	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	10	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	12	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	12	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	12	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	12	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	12	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	12	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	14	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	14	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	14	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	14	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	14	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	14	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	15	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	15	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	15	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	15	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	15	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	15	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	17	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	17	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	17	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	17	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	17	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	17	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	19	0.29
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	19	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	19	0.29
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	19	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	19	0.29
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	19	0.29
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	2	0.28
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	16	0.28
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	16	0.28
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	7	0.28
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	7	0.28
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	15	0.28
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	15	0.28
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	7	0.28
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	7	0.28
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	15	0.28
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	15	0.28
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	17	0.28
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	17	0.28
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	20	0.28
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	20	0.28
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	20	0.28
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	20	0.28
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	20	0.28
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	20	0.28
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	15	0.28
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	15	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	1	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	4	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	5	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	6	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	7	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	9	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	10	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	11	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	12	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	13	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	14	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	15	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	16	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	17	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	18	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	19	0.28
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	20	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	2	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	2	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	7	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	15	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	15	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	16	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	16	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	19	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	19	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	20	0.28
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	20	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	1	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	3	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	4	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	5	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	6	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	8	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	9	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	10	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	11	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	12	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	13	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	14	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	17	0.28
(2,468)	1:12:A:ILE:HA	1:13:A:LEU:HG	18	0.28
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	11	0.28
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	11	0.28
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	18	0.28
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	18	0.28
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	5	0.28
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	5	0.28
(2,346)	1:9:A:ARG:HB2	1:10:A:ASP:HA	14	0.28
(2,346)	1:9:A:ARG:HB3	1:10:A:ASP:HA	14	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD11	16	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD12	16	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD13	16	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD21	16	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD22	16	0.28
(2,266)	1:7:A:PHE:HE1	1:13:A:LEU:HD23	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD11	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD12	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD13	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD21	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD22	16	0.28
(2,266)	1:7:A:PHE:HE2	1:13:A:LEU:HD23	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	3	0.28
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	3	0.28
(2,205)	1:6:A:LYS:HB2	1:10:A:ASP:HA	17	0.28
(2,205)	1:6:A:LYS:HB3	1:10:A:ASP:HA	17	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	2	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	4	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	5	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	13	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	17	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	18	0.28
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	20	0.28
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	1	0.28
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	1	0.28
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	7	0.28
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	7	0.28
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	11	0.28
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	11	0.28
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	5	0.28
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	5	0.28
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	9	0.28
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	9	0.28
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	12	0.28
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	12	0.28
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	5	0.28
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	13	0.28
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	13	0.28
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	13	0.28
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	13	0.28
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	13	0.28
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	13	0.28
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	13	0.28
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	3	0.28
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	3	0.28
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	10	0.28
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	10	0.28
(2,109)	1:4:A:LEU:HD11	1:5:A:SER:HA	5	0.28
(2,109)	1:4:A:LEU:HD12	1:5:A:SER:HA	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:4:A:LEU:HD13	1:5:A:SER:HA	5	0.28
(2,109)	1:4:A:LEU:HD21	1:5:A:SER:HA	5	0.28
(2,109)	1:4:A:LEU:HD22	1:5:A:SER:HA	5	0.28
(2,109)	1:4:A:LEU:HD23	1:5:A:SER:HA	5	0.28
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	5	0.28
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	2	0.28
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	2	0.28
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	9	0.28
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	9	0.28
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB2	2	0.28
(2,38)	1:2:A:MET:HE1	1:5:A:SER:HB3	2	0.28
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB2	2	0.28
(2,38)	1:2:A:MET:HE2	1:5:A:SER:HB3	2	0.28
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB2	2	0.28
(2,38)	1:2:A:MET:HE3	1:5:A:SER:HB3	2	0.28
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB2	2	0.28
(2,37)	1:2:A:MET:HE1	1:5:A:SER:HB3	2	0.28
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB2	2	0.28
(2,37)	1:2:A:MET:HE2	1:5:A:SER:HB3	2	0.28
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB2	2	0.28
(2,37)	1:2:A:MET:HE3	1:5:A:SER:HB3	2	0.28
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	1	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	1	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	4	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	4	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	5	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	5	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	10	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	10	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	11	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	11	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	13	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	13	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	14	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	14	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	17	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	17	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	18	0.27
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	18	0.27
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	19	0.27
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	19	0.27
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	20	0.27
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	7	0.27
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	15	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	1	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	1	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	2	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	2	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	3	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	3	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	4	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	4	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	5	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	5	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	6	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	6	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	7	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	7	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	8	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	8	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	9	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	9	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	10	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	10	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	11	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	11	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	12	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	12	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	13	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	13	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	14	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	14	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	16	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	16	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	17	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	17	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	18	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	18	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	19	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	19	0.27
(2,484)	1:12:A:ILE:HG12	1:14:A:GLN:H	20	0.27
(2,484)	1:12:A:ILE:HG13	1:14:A:GLN:H	20	0.27
(2,480)	1:12:A:ILE:H	1:13:A:LEU:H	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	1	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	1	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	3	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	3	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	4	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	4	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	5	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	5	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	8	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	8	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	10	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	10	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	13	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	13	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	14	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	14	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG2	17	0.27
(2,443)	1:11:A:DPN:HB3	1:14:A:GLN:HG3	17	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	2	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	2	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	3	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	3	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	4	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	4	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	8	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	8	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	9	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	9	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	12	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	12	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	15	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	15	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	17	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	17	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	18	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	18	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	19	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	19	0.27
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	20	0.27
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	20	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	1	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	7	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	7	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	10	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	10	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	11	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	11	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	14	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	14	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	16	0.27
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	16	0.27
(2,204)	1:6:A:LYS:H	1:7:A:PHE:HA	9	0.27
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	19	0.27
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	19	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	2	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	2	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	3	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	3	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	4	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	4	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	6	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	6	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	8	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	8	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	10	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	10	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	11	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	11	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	15	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	15	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	17	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	17	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	18	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	18	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	19	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	19	0.27
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	20	0.27
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	20	0.27
(2,159)	1:4:A:LEU:HD11	1:8:A:PHE:H	5	0.27
(2,159)	1:4:A:LEU:HD12	1:8:A:PHE:H	5	0.27
(2,159)	1:4:A:LEU:HD13	1:8:A:PHE:H	5	0.27
(2,159)	1:4:A:LEU:HD21	1:8:A:PHE:H	5	0.27
(2,159)	1:4:A:LEU:HD22	1:8:A:PHE:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,159)	1:4:A:LEU:HD23	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD11	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD12	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD13	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD21	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD22	1:8:A:PHE:H	5	0.27
(2,154)	1:4:A:LEU:HD23	1:8:A:PHE:H	5	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	13	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	13	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	16	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	16	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	20	0.27
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	20	0.27
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	14	0.27
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	14	0.27
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	6	0.26
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	6	0.26
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	9	0.26
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	9	0.26
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	7	0.26
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	7	0.26
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	7	0.26
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	7	0.26
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	15	0.26
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	15	0.26
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	15	0.26
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	15	0.26
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	2	0.26
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	16	0.26
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	18	0.26
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	19	0.26
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	20	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	1	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	1	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	3	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	3	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	4	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	4	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	5	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	5	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	6	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	8	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	8	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	9	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	9	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	10	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	10	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	11	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	11	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	12	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	12	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	13	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	13	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	14	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	14	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	17	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	17	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB2	18	0.26
(2,476)	1:12:A:ILE:H	1:13:A:LEU:HB3	18	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	1	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	1	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	6	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	6	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	7	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	7	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	10	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	10	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	11	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	11	0.26
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	16	0.26
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	16	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	2	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	2	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	7	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	7	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	15	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	15	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	16	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	16	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	19	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	19	0.26
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	20	0.26
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	2	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	2	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	4	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	4	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	5	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	5	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	6	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	6	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	8	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	8	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	9	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	9	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	12	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	12	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	13	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	13	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	15	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	15	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	17	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	17	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	18	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	18	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	19	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	19	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG2	20	0.26
(2,243)	1:7:A:PHE:H	1:9:A:ARG:HG3	20	0.26
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	15	0.26
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	15	0.26
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	1	0.26
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	1	0.26
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	7	0.26
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	7	0.26
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	13	0.26
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	13	0.26
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	14	0.26
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	14	0.26
(2,196)	1:5:A:SER:HB2	1:9:A:ARG:H	16	0.26
(2,196)	1:5:A:SER:HB3	1:9:A:ARG:H	16	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	1	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	1	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	4	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	6	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	6	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	7	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	7	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	8	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	8	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	11	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	11	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	18	0.26
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	18	0.26
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	3	0.26
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	3	0.26
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	5	0.26
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	5	0.26
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	10	0.26
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	10	0.26
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	1	0.26
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	7	0.26
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	18	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	1	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	1	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	4	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	4	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	6	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	6	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	7	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	7	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	8	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	8	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	11	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	11	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	13	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	13	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	16	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	16	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	18	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	18	0.26
(2,63)	1:3:A:ARG:HG2	1:3:A:ARG:H	20	0.26
(2,63)	1:3:A:ARG:HG3	1:3:A:ARG:H	20	0.26
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	3	0.25
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	3	0.25
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	8	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	2	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	2	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	2	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	2	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	16	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	16	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	16	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	16	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	19	0.25
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	19	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	19	0.25
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	19	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	1	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	4	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	5	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	6	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	9	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	10	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	11	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	12	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	13	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	14	0.25
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	17	0.25
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	3	0.25
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	3	0.25
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	8	0.25
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	8	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	1	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	1	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	1	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	1	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	2	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	2	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	2	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	2	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	3	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	3	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	3	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	3	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	4	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	4	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	4	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	5	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	5	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	5	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	5	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	6	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	6	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	6	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	6	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	7	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	7	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	7	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	7	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	8	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	8	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	8	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	8	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	9	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	9	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	9	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	9	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	10	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	10	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	10	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	10	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	11	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	11	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	11	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	11	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	12	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	12	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	12	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	12	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	13	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	13	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	13	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	13	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	14	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	14	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	14	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	15	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	15	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	15	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	15	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	16	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	16	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	16	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	16	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	17	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	17	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	17	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	17	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	18	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	18	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	18	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	18	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	19	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	19	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	19	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	19	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE1	20	0.25
(2,212)	1:7:A:PHE:HB2	1:7:A:PHE:HE2	20	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE1	20	0.25
(2,212)	1:7:A:PHE:HB3	1:7:A:PHE:HE2	20	0.25
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	12	0.25
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	12	0.25
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	15	0.25
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	15	0.25
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	17	0.25
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	17	0.25
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	19	0.25
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	19	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	4	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	6	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	8	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	11	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	13	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	16	0.25
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	20	0.25
(2,577)	1:17:A:LYS:HB2	1:17:A:LYS:H	12	0.24
(2,577)	1:17:A:LYS:HB3	1:17:A:LYS:H	12	0.24
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	2	0.24
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	16	0.24
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	16	0.24
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	19	0.24
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	19	0.24
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	6	0.24
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	9	0.24
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	12	0.24
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	12	0.24
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	12	0.24
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	12	0.24
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	12	0.24
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	12	0.24
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	3	0.24
(2,485)	1:12:A:ILE:H	1:14:A:GLN:HA	8	0.24
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	6	0.24
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	9	0.24
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	13	0.24
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	13	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	1	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	1	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	4	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	4	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	5	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	5	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	6	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	6	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	9	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	9	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	10	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	10	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	11	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	12	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	12	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	13	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	13	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	14	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	14	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	17	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	17	0.24
(2,319)	1:8:A:PHE:HE1	1:12:A:ILE:H	18	0.24
(2,319)	1:8:A:PHE:HE2	1:12:A:ILE:H	18	0.24
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	3	0.24
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	3	0.24
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	12	0.24
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	12	0.24
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	5	0.24
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	5	0.24
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	5	0.24
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	3	0.24
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	10	0.24
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	12	0.23
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	12	0.23
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	12	0.23
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	12	0.23
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	20	0.23
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	20	0.23
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	20	0.23
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	20	0.23
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	20	0.23
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	20	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	1	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	4	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	4	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	4	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	4	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	4	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	5	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	10	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	11	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	13	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	14	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	17	0.23
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	18	0.23
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	18	0.23
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	18	0.23
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	18	0.23
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	18	0.23
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	2	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	6	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	7	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	9	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	12	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	15	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	16	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	19	0.23
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	20	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	2	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	7	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	15	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	16	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	19	0.23
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	20	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	1	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	3	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	4	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	5	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	8	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	10	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	11	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	12	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	13	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	14	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	17	0.23
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	18	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	1	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	2	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	6	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	7	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	9	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	12	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	14	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	16	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	17	0.23
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	18	0.23
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	5	0.23
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	13	0.23
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	2	0.23
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	16	0.23
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	20	0.23
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	5	0.23
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	5	0.23
(2,340)	1:9:A:ARG:HD2	1:9:A:ARG:H	14	0.23
(2,340)	1:9:A:ARG:HD3	1:9:A:ARG:H	14	0.23
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	5	0.23
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	5	0.23
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	12	0.23
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	12	0.23
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	5	0.23
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	5	0.23
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	12	0.23
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	12	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	1	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	1	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	2	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	2	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	3	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	3	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	3	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	3	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	3	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	3	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	4	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	4	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	6	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	6	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	7	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	7	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	7	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	7	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	7	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	7	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	8	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	8	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	9	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	9	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	10	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	10	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	11	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	11	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	11	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	11	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	11	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	11	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	12	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	12	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	13	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	13	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	14	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	14	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	14	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	14	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	14	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	14	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	15	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	15	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	16	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	16	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	17	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	17	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	18	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	18	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	18	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	18	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	18	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	18	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	19	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	19	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.23
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	1	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	1	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	1	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	1	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	1	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	1	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	2	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	2	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	3	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	3	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	4	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	4	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	6	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	6	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	6	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	6	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	6	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	6	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	7	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	7	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	8	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	8	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	9	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	9	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	9	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	9	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	9	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	9	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	10	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	10	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	11	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	11	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	12	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	12	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	13	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	13	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	13	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	13	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	13	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	13	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	14	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	14	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	15	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	15	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	16	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	16	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	16	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	16	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	16	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	16	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	17	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	17	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	18	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	18	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	19	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	19	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.23
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.23
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.23
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.23
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.23
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.23
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB2	5	0.23
(2,78)	1:3:A:ARG:H	1:4:A:LEU:HB3	5	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	2	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	9	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	12	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	14	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	15	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	17	0.23
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	19	0.23
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	9	0.22
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	9	0.22
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	9	0.22
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	9	0.22
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	3	0.22
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	8	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	1	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	1	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	3	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	3	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	4	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	4	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	5	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	5	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	8	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	8	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	10	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	10	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	11	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	11	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	13	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	13	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	14	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	14	0.22
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	17	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	18	0.22
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	18	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	1	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	1	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	3	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	3	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	4	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	4	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	5	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	5	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	8	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	8	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	10	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	10	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	11	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	11	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	13	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	13	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	14	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	14	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	17	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	17	0.22
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	18	0.22
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	18	0.22
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	3	0.22
(2,524)	1:13:A:LEU:HD11	1:16:A:LYS:HA	8	0.22
(2,524)	1:13:A:LEU:HD12	1:16:A:LYS:HA	8	0.22
(2,524)	1:13:A:LEU:HD13	1:16:A:LYS:HA	8	0.22
(2,524)	1:13:A:LEU:HD21	1:16:A:LYS:HA	8	0.22
(2,524)	1:13:A:LEU:HD22	1:16:A:LYS:HA	8	0.22
(2,524)	1:13:A:LEU:HD23	1:16:A:LYS:HA	8	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	1	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	3	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	4	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	5	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	8	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	11	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	13	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	14	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	17	0.22
(2,521)	1:13:A:LEU:HG	1:15:A:ARG:H	18	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	1	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	2	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	3	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	4	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	5	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	6	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	7	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	8	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	9	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	10	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	11	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	12	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	13	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	14	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	16	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	17	0.22
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	18	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	3	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	4	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	5	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	8	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	10	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	11	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	13	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	15	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	19	0.22
(2,373)	1:10:A:ASP:HA	1:11:A:DPN:HZ	20	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	1	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	3	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	4	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	6	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	8	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	9	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	10	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	11	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	12	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	17	0.22
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	18	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	5	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	7	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	8	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	14	0.22
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	15	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	1	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	1	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	2	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	2	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	3	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	3	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	4	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	4	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	6	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	6	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	7	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	7	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	8	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	8	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	9	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	9	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	10	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	10	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	11	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	11	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	13	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	13	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	14	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	14	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	15	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	15	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	16	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	16	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	17	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	17	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	18	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	18	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	19	0.22
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	19	0.22
(2,295)	1:8:A:PHE:HB2	1:10:A:ASP:H	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:8:A:PHE:HB3	1:10:A:ASP:H	20	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	1	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	1	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	2	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	2	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	3	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	3	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	4	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	4	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	6	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	6	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	7	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	7	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	8	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	8	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	9	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	9	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	10	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	10	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	11	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	11	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	13	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	13	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	14	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	14	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	15	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	15	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	16	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	16	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	17	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	17	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	18	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	18	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	19	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	19	0.22
(2,294)	1:8:A:PHE:HB2	1:10:A:ASP:H	20	0.22
(2,294)	1:8:A:PHE:HB3	1:10:A:ASP:H	20	0.22
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	12	0.22
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	12	0.22
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	17	0.22
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	17	0.22
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	19	0.22
(2,2)	1:2:A:MET:HA	1:2:A:MET:HG2	5	0.22
(2,2)	1:2:A:MET:HA	1:2:A:MET:HG3	5	0.22
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	1	0.21
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	4	0.21
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	12	0.21
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	15	0.21
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	15	0.21
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	7	0.21
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	7	0.21
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	15	0.21
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	15	0.21
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	7	0.21
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	7	0.21
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	15	0.21
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	15	0.21
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	6	0.21
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	6	0.21
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	6	0.21
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	6	0.21
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	9	0.21
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	9	0.21
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	9	0.21
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	9	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	2	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	7	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	15	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	16	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	19	0.21
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	20	0.21
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	6	0.21
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	6	0.21
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	2	0.21
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	15	0.21
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	16	0.21
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	19	0.21
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	20	0.21
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	15	0.21
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	19	0.21
(2,392)	1:10:A:ASP:HA	1:13:A:LEU:H	20	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	1	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	4	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	6	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	9	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	10	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	11	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	12	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	13	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	17	0.21
(2,359)	1:9:A:ARG:HA	1:12:A:ILE:H	18	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	1	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	4	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	6	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	7	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	8	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	11	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	13	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	16	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	18	0.21
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	20	0.21
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD11	1:5:A:SER:HB3	5	0.21
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD12	1:5:A:SER:HB3	5	0.21
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD13	1:5:A:SER:HB3	5	0.21
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD21	1:5:A:SER:HB3	5	0.21
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD22	1:5:A:SER:HB3	5	0.21
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB2	5	0.21
(2,110)	1:4:A:LEU:HD23	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB2	5	0.21
(2,106)	1:4:A:LEU:HD11	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB2	5	0.21
(2,106)	1:4:A:LEU:HD12	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB2	5	0.21
(2,106)	1:4:A:LEU:HD13	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB2	5	0.21
(2,106)	1:4:A:LEU:HD21	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB2	5	0.21
(2,106)	1:4:A:LEU:HD22	1:5:A:SER:HB3	5	0.21
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB2	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:4:A:LEU:HD23	1:5:A:SER:HB3	5	0.21
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	3	0.21
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	10	0.21
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	2	0.21
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	2	0.21
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	9	0.21
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	9	0.21
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	10	0.21
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	10	0.21
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	14	0.21
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	14	0.21
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	15	0.21
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	15	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD11	5	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD12	5	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD13	5	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD21	5	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD22	5	0.21
(2,65)	1:3:A:ARG:HA	1:4:A:LEU:HD23	5	0.21
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE1	5	0.21
(2,42)	1:2:A:MET:HB2	1:7:A:PHE:HE2	5	0.21
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE1	5	0.21
(2,42)	1:2:A:MET:HB3	1:7:A:PHE:HE2	5	0.21
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	6	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	6	0.2
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	11	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	11	0.2
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	13	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	13	0.2
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	17	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	17	0.2
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	18	0.2
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	18	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	5	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	6	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	9	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	10	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	11	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	13	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	14	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	17	0.2
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	19	0.2
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	19	0.2
(2,555)	1:15:A:ARG:HD2	1:16:A:LYS:HA	7	0.2
(2,555)	1:15:A:ARG:HD3	1:16:A:LYS:HA	7	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	2	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	2	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	6	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	6	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	9	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	9	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	12	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	12	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	16	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	16	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	19	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	19	0.2
(2,538)	1:14:A:GLN:HB2	1:15:A:ARG:HA	20	0.2
(2,538)	1:14:A:GLN:HB3	1:15:A:ARG:HA	20	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	2	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	2	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	6	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	6	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	9	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	9	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	12	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	12	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	16	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	16	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	19	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	19	0.2
(2,536)	1:14:A:GLN:HB2	1:15:A:ARG:HA	20	0.2
(2,536)	1:14:A:GLN:HB3	1:15:A:ARG:HA	20	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	1	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	1	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	1	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	1	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	3	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	3	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	3	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	3	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	4	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	4	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	4	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	5	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	5	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	5	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	5	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	8	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	8	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	8	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	8	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	10	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	10	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	10	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	10	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	11	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	11	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	11	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	11	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	12	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	12	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	12	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	12	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	13	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	13	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	13	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	13	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	14	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	14	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	14	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	14	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	17	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	17	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	17	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	17	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	18	0.2
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	18	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	18	0.2
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	18	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	1	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	1	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	3	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	4	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	4	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	5	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	5	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	8	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	8	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	9	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	9	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	10	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	10	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	11	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	11	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	12	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	12	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	13	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	13	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	14	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	14	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	17	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	17	0.2
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	18	0.2
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	18	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	1	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	3	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	4	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	5	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	6	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	8	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	9	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	10	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	11	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	12	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	13	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	14	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	17	0.2
(2,469)	1:12:A:ILE:HA	1:13:A:LEU:H	18	0.2
(2,450)	1:11:A:DPN:HZ	1:14:A:GLN:H	7	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	1	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	3	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	4	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	5	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	8	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	9	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	10	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	11	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	12	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	13	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	14	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	17	0.2
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	18	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	1	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	1	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	2	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	2	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	3	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	3	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	4	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	4	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	5	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	5	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	6	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	6	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	7	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	7	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	8	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	8	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	9	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	9	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	10	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	10	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	11	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	11	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	12	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	12	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	13	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	13	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	14	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	14	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	15	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	15	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	16	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	16	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	17	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	18	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	18	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	19	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	19	0.2
(2,246)	1:7:A:PHE:HB2	1:10:A:ASP:H	20	0.2
(2,246)	1:7:A:PHE:HB3	1:10:A:ASP:H	20	0.2
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	3	0.2
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	3	0.2
(2,47)	1:3:A:ARG:HA	1:3:A:ARG:HD2	5	0.2
(2,47)	1:3:A:ARG:HA	1:3:A:ARG:HD3	5	0.2
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	7	0.19
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	7	0.19
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	15	0.19
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	15	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	1	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	1	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	3	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	3	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	4	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	4	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	5	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	5	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	8	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	8	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	9	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	9	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	10	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	10	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	12	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	12	0.19
(2,570)	1:16:A:LYS:HB2	1:17:A:LYS:H	14	0.19
(2,570)	1:16:A:LYS:HB3	1:17:A:LYS:H	14	0.19
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	6	0.19
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	6	0.19
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	6	0.19
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	6	0.19
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	2	0.19
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	2	0.19
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	16	0.19
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	16	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	2	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	2	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	2	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	7	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	7	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	7	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	7	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	15	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	15	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	15	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	15	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	16	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	16	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	16	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	16	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	19	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	19	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	19	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	19	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE21	20	0.19
(2,508)	1:13:A:LEU:HB2	1:14:A:GLN:HE22	20	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE21	20	0.19
(2,508)	1:13:A:LEU:HB3	1:14:A:GLN:HE22	20	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	1	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	1	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	1	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	1	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	1	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	1	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	3	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	3	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	3	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	3	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	3	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	3	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	4	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	4	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	4	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	4	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	4	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	4	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	5	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	5	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	5	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	5	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	5	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	8	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	8	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	8	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	8	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	8	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	8	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	10	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	10	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	10	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	10	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	10	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	10	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	11	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	11	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	11	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	11	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	11	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	11	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	13	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	13	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	13	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	13	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	13	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	13	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	14	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	14	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	14	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	14	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	14	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	14	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	17	0.19
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	17	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	17	0.19
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	17	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	17	0.19
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	17	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	3	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	4	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	5	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	6	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	8	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	9	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	10	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	11	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	12	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	13	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	14	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	17	0.19
(2,475)	1:12:A:ILE:H	1:13:A:LEU:HA	18	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	2	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	7	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	15	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	16	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	19	0.19
(2,365)	1:9:A:ARG:H	1:13:A:LEU:H	20	0.19
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	1	0.19
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	1	0.19
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	16	0.19
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	16	0.19
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	17	0.19
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	17	0.19
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	3	0.19
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	9	0.19
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	10	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	1	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	1	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	1	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	1	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	2	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	2	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	2	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	2	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	4	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	4	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	4	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	4	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	6	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	6	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	6	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	7	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	7	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	7	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	7	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	8	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	8	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	8	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	8	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	11	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	11	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	11	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	11	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	12	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	12	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	12	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	12	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	13	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	13	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	13	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	13	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	14	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	14	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	14	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	14	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	16	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	16	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	16	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	16	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	18	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	18	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	18	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	18	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	20	0.19
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	20	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	20	0.19
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	20	0.19
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	20	0.18
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	20	0.18
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	19	0.18
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	19	0.18
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	19	0.18
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	20	0.18
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	20	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	6	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	6	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	6	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	6	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	6	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	6	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	9	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	9	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	9	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	9	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	9	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	9	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	12	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	12	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	12	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	12	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	12	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	12	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	18	0.18
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	18	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	18	0.18
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	18	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	18	0.18
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	18	0.18
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	5	0.18
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	5	0.18
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	18	0.18
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	18	0.18
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	5	0.18
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	5	0.18
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	18	0.18
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	18	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	1	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	3	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	4	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	6	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	8	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	10	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	11	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	12	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	13	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	14	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	17	0.18
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	18	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	2	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	2	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	3	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	3	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	4	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	4	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	5	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	5	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	6	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	6	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	7	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	7	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	8	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	8	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	9	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	9	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	10	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	10	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	11	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	11	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	12	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	12	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	13	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	13	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	14	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	14	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	15	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	15	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	18	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	18	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	19	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	19	0.18
(2,248)	1:7:A:PHE:HD1	1:10:A:ASP:H	20	0.18
(2,248)	1:7:A:PHE:HD2	1:10:A:ASP:H	20	0.18
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	14	0.18
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	15	0.18
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	19	0.18
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD1	5	0.18
(2,138)	1:4:A:LEU:H	1:7:A:PHE:HD2	5	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	9	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	9	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	9	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	9	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	15	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	15	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	15	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	15	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	17	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	17	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	17	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	17	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	19	0.18
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	19	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	19	0.18
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	19	0.18
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	2	0.18
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	2	0.18
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	9	0.18
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	9	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	1	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	1	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	4	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	4	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	6	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	6	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	7	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	7	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	8	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	8	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	11	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	11	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	13	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	13	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	16	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	16	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	18	0.18
(2,68)	1:3:A:ARG:HB2	1:4:A:LEU:HA	20	0.18
(2,68)	1:3:A:ARG:HB3	1:4:A:LEU:HA	20	0.18
(2,34)	1:2:A:MET:HB2	1:5:A:SER:HB2	5	0.18
(2,34)	1:2:A:MET:HB2	1:5:A:SER:HB3	5	0.18
(2,34)	1:2:A:MET:HB3	1:5:A:SER:HB2	5	0.18
(2,34)	1:2:A:MET:HB3	1:5:A:SER:HB3	5	0.18
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	1	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	1	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	4	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	4	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	5	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	5	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	6	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	6	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	9	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	9	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	10	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	10	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	11	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	11	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	13	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	13	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	14	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	14	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	17	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	17	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	18	0.17
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	18	0.17
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	16	0.17
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	16	0.17
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	16	0.17
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	16	0.17
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	7	0.17
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	7	0.17
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	15	0.17
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	15	0.17
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	15	0.17
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	7	0.17
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	7	0.17
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	7	0.17
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	7	0.17
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	7	0.17
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	2	0.17
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	2	0.17
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	7	0.17
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	7	0.17
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	15	0.17
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	15	0.17
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	20	0.17
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	20	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	1	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	1	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	1	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	3	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	3	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	3	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	4	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	4	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	4	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	5	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	5	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	5	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	6	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	6	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	6	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	7	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	7	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	7	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	8	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	8	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	8	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	9	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	9	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	9	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	10	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	10	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	10	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	11	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	11	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	11	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	12	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	12	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	13	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	13	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	13	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	14	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	14	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	14	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	17	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	17	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	17	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	18	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	18	0.17
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	18	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	3	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	3	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	4	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	4	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	6	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	6	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	8	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	8	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	9	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	9	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	10	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	10	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	11	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	11	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	12	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	12	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	13	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	13	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	15	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	15	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	19	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	19	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	20	0.17
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	20	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	3	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	3	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	4	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	4	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	6	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	8	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	8	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	9	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	9	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	10	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	10	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	11	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	11	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	12	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	12	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	13	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	13	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	15	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	15	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	19	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	19	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	20	0.17
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	20	0.17
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	7	0.17
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	15	0.17
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	5	0.17
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	5	0.17
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	5	0.17
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	18	0.17
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	18	0.17
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	12	0.17
(2,165)	1:4:A:LEU:H	1:9:A:ARG:H	17	0.17
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	3	0.17
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	3	0.17
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	3	0.17
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	3	0.17
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE1	10	0.17
(2,88)	1:3:A:ARG:HB2	1:7:A:PHE:HE2	10	0.17
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE1	10	0.17
(2,88)	1:3:A:ARG:HB3	1:7:A:PHE:HE2	10	0.17
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	14	0.17
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	14	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	1	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	1	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	4	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	6	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	6	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	7	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	7	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	8	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	8	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	11	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	11	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	13	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	13	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	16	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	16	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	18	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	18	0.17
(2,74)	1:3:A:ARG:HD2	1:4:A:LEU:H	20	0.17
(2,74)	1:3:A:ARG:HD3	1:4:A:LEU:H	20	0.17
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	7	0.16
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	7	0.16
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	15	0.16
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	15	0.16
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	20	0.16
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	20	0.16
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	3	0.16
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	3	0.16
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	8	0.16
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	8	0.16
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	12	0.16
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	12	0.16
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	2	0.16
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	2	0.16
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	16	0.16
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	16	0.16
(2,578)	1:17:A:LYS:HD2	1:17:A:LYS:H	19	0.16
(2,578)	1:17:A:LYS:HD3	1:17:A:LYS:H	19	0.16
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	3	0.16
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	3	0.16
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	8	0.16
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	8	0.16
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	2	0.16
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	2	0.16
(2,566)	1:16:A:LYS:HB2	1:16:A:LYS:H	20	0.16
(2,566)	1:16:A:LYS:HB3	1:16:A:LYS:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	2	0.16
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	2	0.16
(2,565)	1:16:A:LYS:HB2	1:16:A:LYS:H	20	0.16
(2,565)	1:16:A:LYS:HB3	1:16:A:LYS:H	20	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	7	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	7	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	15	0.16
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	15	0.16
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE2	12	0.16
(2,559)	1:15:A:ARG:HB2	1:17:A:LYS:HE3	12	0.16
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE2	12	0.16
(2,559)	1:15:A:ARG:HB3	1:17:A:LYS:HE3	12	0.16
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	6	0.16
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	6	0.16
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	19	0.16
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	19	0.16
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	20	0.16
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	20	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	1	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	2	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	3	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	4	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	5	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	6	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	7	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	8	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	9	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	10	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	11	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	12	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	13	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	14	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	16	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	17	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	18	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	19	0.16
(2,516)	1:13:A:LEU:HG	1:14:A:GLN:H	20	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	1	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	3	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	4	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	5	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	8	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	10	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	11	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	12	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	13	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	14	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	17	0.16
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	18	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	2	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	2	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	2	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	2	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	2	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	2	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	15	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	15	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	15	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	15	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	15	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	15	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	16	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	16	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	16	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	16	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	16	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	16	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	19	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	19	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	19	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	19	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	19	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	19	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE21	20	0.16
(2,481)	1:12:A:ILE:HD11	1:14:A:GLN:HE22	20	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE21	20	0.16
(2,481)	1:12:A:ILE:HD12	1:14:A:GLN:HE22	20	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE21	20	0.16
(2,481)	1:12:A:ILE:HD13	1:14:A:GLN:HE22	20	0.16
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	16	0.16
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	16	0.16
(2,474)	1:12:A:ILE:HG12	1:13:A:LEU:H	19	0.16
(2,474)	1:12:A:ILE:HG13	1:13:A:LEU:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	2	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	2	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	2	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	15	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	15	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	15	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	16	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	16	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	16	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	19	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	19	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	19	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD11	20	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD12	20	0.16
(2,455)	1:12:A:ILE:HA	1:12:A:ILE:HD13	20	0.16
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	7	0.16
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	15	0.16
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	19	0.16
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	20	0.16
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	2	0.16
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	16	0.16
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	19	0.16
(2,327)	1:8:A:PHE:H	1:13:A:LEU:H	20	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	2	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	7	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	15	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	16	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	19	0.16
(2,311)	1:8:A:PHE:HA	1:12:A:ILE:HB	20	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	5	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	5	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	5	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	5	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	13	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	13	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	13	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	13	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	14	0.16
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	14	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	14	0.16
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	14	0.16
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	5	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	5	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	5	0.16
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	8	0.16
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	8	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	8	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	8	0.16
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	18	0.16
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	18	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	18	0.16
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	18	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	1	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	1	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	2	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	2	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	3	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	3	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	4	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	4	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	6	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	6	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	7	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	7	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	8	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	8	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	9	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	9	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	10	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	10	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	11	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	11	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	12	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	12	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	13	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	13	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	14	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	14	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	15	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	15	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	16	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	16	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	17	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	19	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	19	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD1	20	0.16
(2,171)	1:5:A:SER:HA	1:7:A:PHE:HD2	20	0.16
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	5	0.16
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	5	0.16
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	5	0.16
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	5	0.16
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	5	0.16
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	5	0.16
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	5	0.16
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	2	0.16
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	17	0.16
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	3	0.16
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	3	0.16
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	5	0.16
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	5	0.16
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	10	0.16
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	10	0.16
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	2	0.16
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	2	0.16
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	9	0.16
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	9	0.16
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	14	0.16
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	14	0.16
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	15	0.16
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	15	0.16
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	19	0.16
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	19	0.16
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	2	0.16
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	2	0.16
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	9	0.16
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	9	0.16
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	14	0.16
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	14	0.16
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	15	0.16
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	19	0.16
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	19	0.16
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	2	0.15
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	2	0.15
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	16	0.15
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	16	0.15
(2,580)	1:17:A:LYS:HG2	1:17:A:LYS:H	19	0.15
(2,580)	1:17:A:LYS:HG3	1:17:A:LYS:H	19	0.15
(2,568)	1:16:A:LYS:HG2	1:16:A:LYS:H	6	0.15
(2,568)	1:16:A:LYS:HG3	1:16:A:LYS:H	6	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	1	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	1	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	2	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	2	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	3	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	3	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	4	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	4	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	5	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	5	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	8	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	8	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	9	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	9	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	10	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	10	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	12	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	12	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	13	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	13	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	14	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	14	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	16	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	16	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	17	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	17	0.15
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	18	0.15
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	18	0.15
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	3	0.15
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	3	0.15
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	8	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	2	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	7	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	9	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	15	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	16	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	19	0.15
(2,493)	1:13:A:LEU:HA	1:13:A:LEU:HG	20	0.15
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	2	0.15
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	16	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	1	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	1	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	2	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	2	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	3	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	3	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	4	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	4	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	5	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	5	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	6	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	6	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	7	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	7	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	8	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	8	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	9	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	9	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	10	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	10	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	11	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	11	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	12	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	12	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	13	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	13	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	14	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	14	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	15	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	15	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	16	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	17	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	17	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	18	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	18	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	19	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	19	0.15
(2,380)	1:10:A:ASP:HB2	1:11:A:DPN:H	20	0.15
(2,380)	1:10:A:ASP:HB3	1:11:A:DPN:H	20	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	1	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	1	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	2	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	2	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	3	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	3	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	4	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	4	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	5	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	5	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	6	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	6	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	7	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	7	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	8	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	8	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	9	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	9	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	10	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	10	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	11	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	11	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	12	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	12	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	13	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	13	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	14	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	14	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	15	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	15	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	16	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	16	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	17	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	18	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	18	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	19	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	19	0.15
(2,376)	1:10:A:ASP:HB2	1:11:A:DPN:H	20	0.15
(2,376)	1:10:A:ASP:HB3	1:11:A:DPN:H	20	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	1	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	2	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	3	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	4	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	5	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	6	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	7	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	8	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	9	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	10	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	11	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	12	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	13	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	14	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	15	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	16	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	17	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	18	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	19	0.15
(2,372)	1:10:A:ASP:HA	1:11:A:DPN:H	20	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	1	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	1	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	14	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	14	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	17	0.15
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	17	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	1	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	1	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	14	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	14	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	17	0.15
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	17	0.15
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	4	0.15
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	4	0.15
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	4	0.15
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	1	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	2	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	3	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	4	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	5	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	6	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	7	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	8	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	9	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	10	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	11	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	12	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	13	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	14	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	15	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	16	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	17	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	18	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	19	0.15
(2,282)	1:8:A:PHE:HA	1:9:A:ARG:H	20	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	1	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	1	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	1	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	1	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	3	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	3	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	3	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	3	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	4	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	4	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	4	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	4	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	6	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	6	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	6	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	6	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	9	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	9	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	9	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	9	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	10	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	10	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	10	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	11	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	11	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	11	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	11	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	12	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	12	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	12	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	12	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	13	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	13	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	13	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	13	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	14	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	14	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	14	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	14	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	17	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	17	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	17	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	17	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	20	0.15
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	20	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	20	0.15
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	20	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	1	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	6	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	7	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	8	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	11	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	16	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	18	0.15
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	20	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	9	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	12	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	14	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	15	0.15
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	19	0.15
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	12	0.15
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	12	0.15
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	15	0.15
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	17	0.15
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	17	0.15
(2,76)	1:3:A:ARG:HD2	1:4:A:LEU:H	19	0.15
(2,76)	1:3:A:ARG:HD3	1:4:A:LEU:H	19	0.15
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	12	0.15
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	12	0.15
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	17	0.15
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	17	0.15
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	12	0.15
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	12	0.15
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	17	0.15
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	17	0.15
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	12	0.15
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	12	0.15
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	12	0.15
(2,568)	1:16:A:LYS:HG2	1:16:A:LYS:H	9	0.14
(2,568)	1:16:A:LYS:HG3	1:16:A:LYS:H	9	0.14
(2,568)	1:16:A:LYS:HG2	1:16:A:LYS:H	12	0.14
(2,568)	1:16:A:LYS:HG3	1:16:A:LYS:H	12	0.14
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	7	0.14
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	15	0.14
(2,557)	1:15:A:ARG:HG2	1:16:A:LYS:H	11	0.14
(2,557)	1:15:A:ARG:HG3	1:16:A:LYS:H	11	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	2	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	2	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	16	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	16	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	19	0.14
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	19	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	1	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	2	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	2	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	2	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	2	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	2	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	3	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	4	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	5	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	6	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	7	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	8	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	9	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	9	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	9	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	9	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	9	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	10	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	11	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	12	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	13	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	14	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	15	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	16	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	16	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	16	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	16	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	16	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	17	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	18	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	19	0.14
(2,511)	1:13:A:LEU:HD11	1:14:A:GLN:H	20	0.14
(2,511)	1:13:A:LEU:HD12	1:14:A:GLN:H	20	0.14
(2,511)	1:13:A:LEU:HD13	1:14:A:GLN:H	20	0.14
(2,511)	1:13:A:LEU:HD21	1:14:A:GLN:H	20	0.14
(2,511)	1:13:A:LEU:HD22	1:14:A:GLN:H	20	0.14
(2,511)	1:13:A:LEU:HD23	1:14:A:GLN:H	20	0.14
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	6	0.14
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	6	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	1	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	3	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	4	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	5	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	6	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	8	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	9	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	10	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	11	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	12	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	13	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	14	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	17	0.14
(2,395)	1:10:A:ASP:H	1:13:A:LEU:HG	18	0.14
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	2	0.14
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	7	0.14
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	7	0.14
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB2	16	0.14
(2,349)	1:9:A:ARG:H	1:10:A:ASP:HB3	16	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	2	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	2	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	7	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	7	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB2	16	0.14
(2,348)	1:9:A:ARG:H	1:10:A:ASP:HB3	16	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	1	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	1	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	1	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	1	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	2	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	2	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	2	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	2	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	6	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	6	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	6	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	6	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	7	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	7	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	7	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	7	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	8	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	8	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	8	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	8	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	9	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	9	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	9	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	9	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	11	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	11	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	11	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	11	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	12	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	12	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	12	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	15	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	15	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	15	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	15	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	16	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	16	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	16	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	16	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	17	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	17	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	17	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	17	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	18	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	18	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	18	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	18	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	19	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	19	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	19	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	19	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	20	0.14
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	20	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	20	0.14
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	20	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	1	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	1	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	2	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	2	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	3	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	3	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	4	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	4	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	6	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	6	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	7	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	7	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	8	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	8	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	9	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	9	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	10	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	11	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	11	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	12	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	12	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	13	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	13	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	14	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	14	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	15	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	15	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	16	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	16	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	17	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	17	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	18	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	18	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	19	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	19	0.14
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	20	0.14
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	20	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	2	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	2	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	2	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	2	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	7	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	7	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	7	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	7	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	15	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	15	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	15	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	15	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	16	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	16	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	16	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	16	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB2	19	0.14
(2,229)	1:7:A:PHE:HD1	1:8:A:PHE:HB3	19	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB2	19	0.14
(2,229)	1:7:A:PHE:HD2	1:8:A:PHE:HB3	19	0.14
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	6	0.14
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	8	0.14
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	8	0.14
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	10	0.14
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	10	0.14
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	14	0.14
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	14	0.14
(2,202)	1:6:A:LYS:HD2	1:6:A:LYS:H	16	0.14
(2,202)	1:6:A:LYS:HD3	1:6:A:LYS:H	16	0.14
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	4	0.14
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	13	0.14
(2,67)	1:3:A:ARG:HA	1:4:A:LEU:H	5	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	1	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	3	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	4	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	8	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	10	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	11	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	13	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	16	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	18	0.14
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	20	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	1	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	1	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	3	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	3	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	6	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	6	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	7	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	7	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	8	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	8	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	10	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	10	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	11	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	11	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	16	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	16	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	18	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	18	0.14
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	20	0.14
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	20	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	1	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	3	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	3	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	6	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	6	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	7	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	7	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	8	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	8	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	10	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	10	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	11	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	11	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	16	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	16	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	18	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	18	0.14
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	20	0.14
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	20	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	1	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	1	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	1	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	2	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	2	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	2	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	3	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	3	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	3	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	4	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	4	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	4	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	6	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	6	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	6	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	7	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	7	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	7	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	8	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	8	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	8	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	9	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	9	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	10	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	10	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	10	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	11	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	11	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	11	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	13	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	13	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	13	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	14	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	14	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	14	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	15	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	15	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	15	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	16	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	16	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	16	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	17	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	17	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	17	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	18	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	18	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	18	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	19	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	19	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	19	0.14
(2,12)	1:2:A:MET:HE1	1:3:A:ARG:H	20	0.14
(2,12)	1:2:A:MET:HE2	1:3:A:ARG:H	20	0.14
(2,12)	1:2:A:MET:HE3	1:3:A:ARG:H	20	0.14
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG2	12	0.13
(2,574)	1:17:A:LYS:HA	1:17:A:LYS:HG3	12	0.13
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	2	0.13
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	16	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	1	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	1	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	4	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	4	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	5	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	5	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	6	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	9	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	9	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	10	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	10	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	11	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	11	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	13	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	13	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	14	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	14	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	17	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	17	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	18	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	18	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	20	0.13
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	20	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	1	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	1	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	2	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	2	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	3	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	3	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	4	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	4	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	5	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	5	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	7	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	7	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	8	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	8	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	9	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	9	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	10	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	10	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	11	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	11	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	12	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	12	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	13	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	13	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	14	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	15	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	15	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	16	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	16	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	17	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	17	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	18	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	18	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	19	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	19	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG12	20	0.13
(2,456)	1:12:A:ILE:HA	1:12:A:ILE:HG13	20	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	1	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	1	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	1	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	2	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	2	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	2	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	3	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	3	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	3	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	4	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	4	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	4	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	5	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	5	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	5	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	6	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	6	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	6	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	8	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	8	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	8	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	9	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	9	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	9	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	10	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	10	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	10	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	11	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	11	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	12	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	12	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	12	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	13	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	13	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	13	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	14	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	14	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	14	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	15	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	15	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	15	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	16	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	16	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	16	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	17	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	17	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	17	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	18	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	18	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	18	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	19	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	19	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	19	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	20	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	20	0.13
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	20	0.13
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	3	0.13
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	3	0.13
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	3	0.13
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	3	0.13
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB2	10	0.13
(2,286)	1:8:A:PHE:HE1	1:9:A:ARG:HB3	10	0.13
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB2	10	0.13
(2,286)	1:8:A:PHE:HE2	1:9:A:ARG:HB3	10	0.13
(2,279)	1:8:A:PHE:HE1	1:8:A:PHE:H	5	0.13
(2,279)	1:8:A:PHE:HE2	1:8:A:PHE:H	5	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	1	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	1	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	2	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	3	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	3	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	4	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	4	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	6	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	6	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	7	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	7	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	8	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	8	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	9	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	9	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	10	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	10	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	11	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	11	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	12	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	12	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	13	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	13	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	15	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	15	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	16	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	16	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	17	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	17	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	18	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	18	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	19	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	19	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	20	0.13
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	20	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	2	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	3	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	3	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	3	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	3	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	3	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	9	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	10	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	12	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	15	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	17	0.13
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	19	0.13
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	19	0.13
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	19	0.13
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	19	0.13
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	19	0.13
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	19	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	2	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	2	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	2	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	2	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	2	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	3	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	9	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	10	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	12	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	15	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	17	0.13
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	19	0.13
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	19	0.13
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	19	0.13
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	19	0.13
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	19	0.13
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	3	0.13
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	10	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	1	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	1	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	2	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	2	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	3	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	3	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	4	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	4	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	4	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	4	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	4	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	4	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	6	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	6	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	7	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	7	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	8	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	8	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	8	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	8	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	8	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	8	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	9	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	9	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	10	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	10	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	11	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	11	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	12	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	12	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	12	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	12	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	12	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	12	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	13	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	13	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	14	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	14	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	15	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	15	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	15	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	15	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	15	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	15	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	16	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	16	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	17	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	17	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	18	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	18	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	19	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	19	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	19	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	19	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	19	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	19	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.13
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	1	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	1	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	2	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	2	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	2	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	2	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	2	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	2	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	3	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	3	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	4	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	4	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	6	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	6	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	7	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	7	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	7	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	7	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	7	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	7	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	8	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	8	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	9	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	9	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	10	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	10	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	10	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	10	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	10	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	10	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	11	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	11	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	12	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	12	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	13	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	13	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	14	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	14	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	14	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	14	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	14	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	14	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	15	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	15	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	16	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	16	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	17	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	17	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	17	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	17	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	17	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	17	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	18	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	18	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	19	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	19	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	20	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	20	0.13
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	20	0.13
(2,81)	1:3:A:ARG:HA	1:5:A:SER:H	5	0.13
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:2:A:MET:HA	1:5:A:SER:H	7	0.13
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	4	0.13
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	4	0.13
(2,30)	1:2:A:MET:HG2	1:4:A:LEU:H	13	0.13
(2,30)	1:2:A:MET:HG3	1:4:A:LEU:H	13	0.13
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	4	0.13
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	4	0.13
(2,27)	1:2:A:MET:HG2	1:4:A:LEU:H	13	0.13
(2,27)	1:2:A:MET:HG3	1:4:A:LEU:H	13	0.13
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	19	0.12
(2,561)	1:15:A:ARG:H	1:17:A:LYS:H	20	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	7	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	7	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	12	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	12	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD2	15	0.12
(2,544)	1:14:A:GLN:H	1:15:A:ARG:HD3	15	0.12
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD11	7	0.12
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD12	7	0.12
(2,387)	1:10:A:ASP:H	1:12:A:ILE:HD13	7	0.12
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	5	0.12
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	5	0.12
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE1	14	0.12
(2,219)	1:7:A:PHE:HA	1:8:A:PHE:HE2	14	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	1	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	4	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	6	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	6	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	6	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	6	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	6	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	7	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	8	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	11	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	14	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	16	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	18	0.12
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	20	0.12
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	20	0.12
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	20	0.12
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	20	0.12
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	20	0.12
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	1	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	4	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	6	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	7	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	8	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	11	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	14	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	14	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	14	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	14	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	14	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	16	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	18	0.12
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	20	0.12
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	20	0.12
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	20	0.12
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	20	0.12
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	20	0.12
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	20	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	3	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	3	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	9	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	9	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	9	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	9	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	9	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	9	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	10	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	10	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	12	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	12	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	15	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	15	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	17	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	17	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	17	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	17	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	17	0.12
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	17	0.12
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	2	0.12
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	9	0.12
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	14	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	1	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	4	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	6	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	7	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	8	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	11	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	13	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	16	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	18	0.12
(2,80)	1:3:A:ARG:H	1:4:A:LEU:H	20	0.12
(2,53)	1:3:A:ARG:HB2	1:3:A:ARG:HE	14	0.12
(2,53)	1:3:A:ARG:HB3	1:3:A:ARG:HE	14	0.12
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	13	0.11
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	13	0.11
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	17	0.11
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	17	0.11
(2,160)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	13	0.11
(2,160)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	13	0.11
(2,160)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	13	0.11
(2,160)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	13	0.11
(2,160)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	13	0.11
(2,160)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD11	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD12	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD13	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD21	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD22	1:8:A:PHE:HZ	13	0.11
(2,155)	1:4:A:LEU:HD23	1:8:A:PHE:HZ	13	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	2	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	2	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	2	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	2	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	2	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	2	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	14	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	14	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	19	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	19	0.11
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	19	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	19	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	19	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	19	0.11
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	19	0.11
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	12	0.11
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	15	0.11
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	17	0.11
(2,114)	1:4:A:LEU:H	1:5:A:SER:HA	19	0.11
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB2	5	0.11
(2,111)	1:4:A:LEU:HD11	1:5:A:SER:HB3	5	0.11
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB2	5	0.11
(2,111)	1:4:A:LEU:HD12	1:5:A:SER:HB3	5	0.11
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB2	5	0.11
(2,111)	1:4:A:LEU:HD13	1:5:A:SER:HB3	5	0.11
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:4:A:LEU:HD21	1:5:A:SER:HB3	5	0.11
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB2	5	0.11
(2,111)	1:4:A:LEU:HD22	1:5:A:SER:HB3	5	0.11
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB2	5	0.11
(2,111)	1:4:A:LEU:HD23	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD11	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD12	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD13	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD21	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD22	1:5:A:SER:HB3	5	0.11
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB2	5	0.11
(2,107)	1:4:A:LEU:HD23	1:5:A:SER:HB3	5	0.11
(2,53)	1:3:A:ARG:HB2	1:3:A:ARG:HE	9	0.11
(2,53)	1:3:A:ARG:HB3	1:3:A:ARG:HE	9	0.11
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	1	0.1
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	1	0.1
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	10	0.1
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	10	0.1
(2,579)	1:17:A:LYS:HE2	1:17:A:LYS:H	14	0.1
(2,579)	1:17:A:LYS:HE3	1:17:A:LYS:H	14	0.1
(2,567)	1:16:A:LYS:HD2	1:16:A:LYS:H	20	0.1
(2,567)	1:16:A:LYS:HD3	1:16:A:LYS:H	20	0.1
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	11	0.1
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	11	0.1
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD2	18	0.1
(2,560)	1:15:A:ARG:HE	1:17:A:LYS:HD3	18	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	1	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	1	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	1	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	1	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	1	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	1	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	8	0.1
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	8	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD11	1:7:A:PHE:HE2	13	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD12	1:7:A:PHE:HE2	13	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD13	1:7:A:PHE:HE2	13	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD21	1:7:A:PHE:HE2	13	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD22	1:7:A:PHE:HE2	13	0.1
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE1	13	0.1
(2,134)	1:4:A:LEU:HD23	1:7:A:PHE:HE2	13	0.1

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

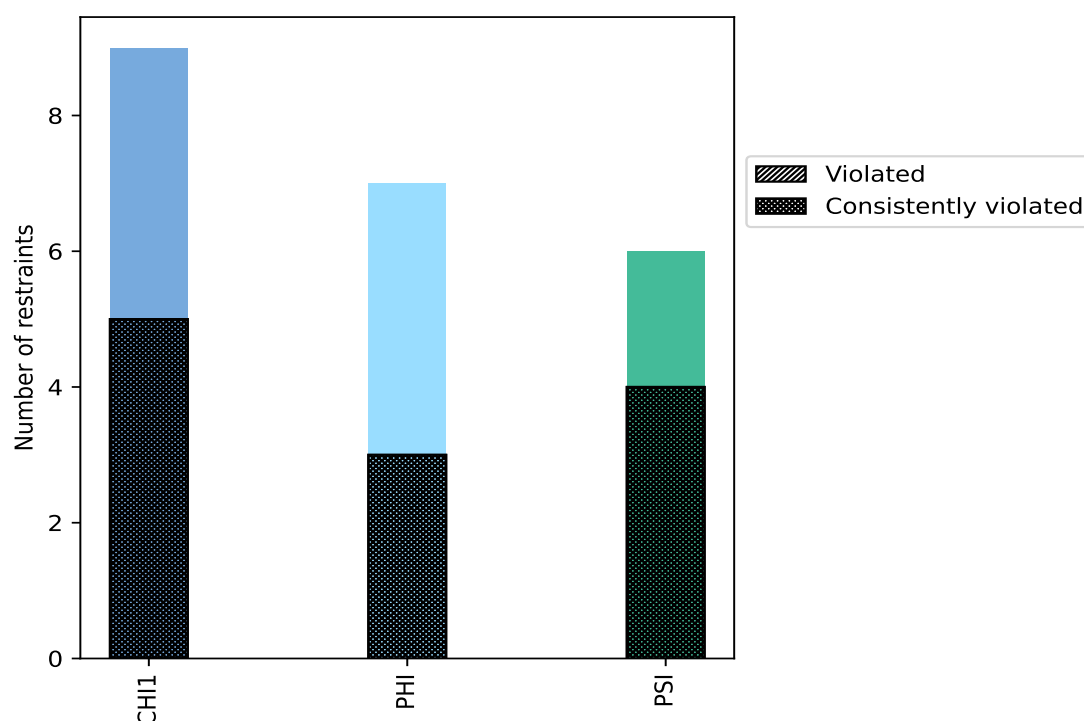
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
CHI1	9	40.9	5	55.6	22.7	5	55.6	22.7
PHI	7	31.8	3	42.9	13.6	3	42.9	13.6
PSI	6	27.3	4	66.7	18.2	4	66.7	18.2
Total	22	100.0	12	54.5	54.5	12	54.5	54.5

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

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



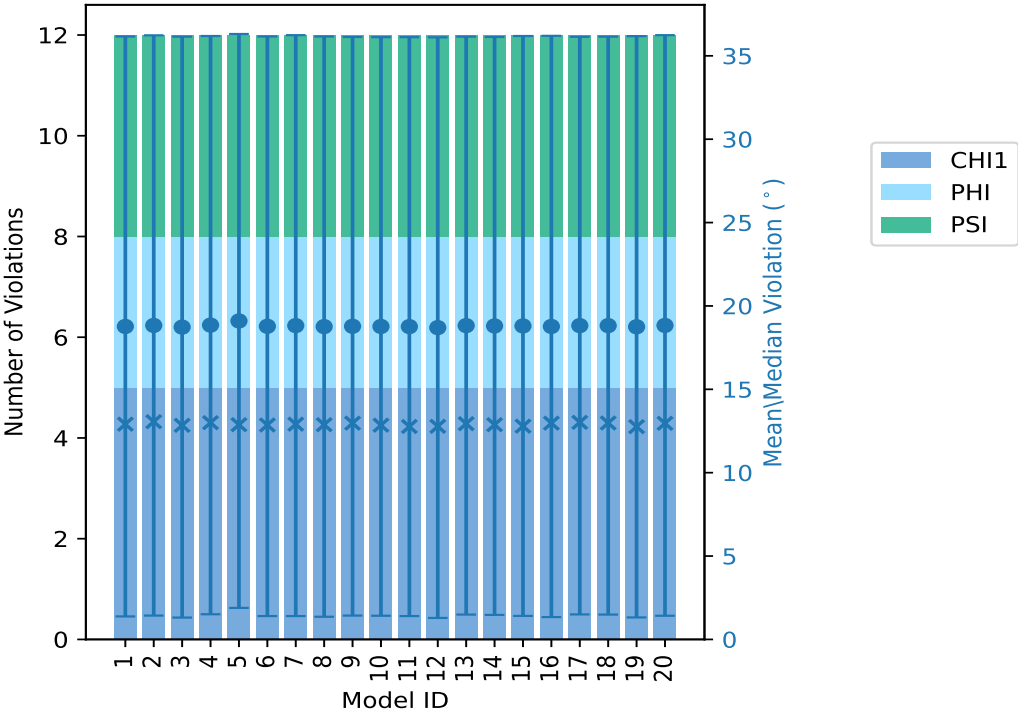
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	CHI1	PHI	PSI	Total				
1	5	3	4	12	18.77	63.08	17.39	12.91
2	5	3	4	12	18.83	63.09	17.4	13.06
3	5	3	4	12	18.73	63.08	17.42	12.84
4	5	3	4	12	18.85	63.11	17.34	13.0
5	5	3	4	12	19.1	62.86	17.21	12.88
6	5	3	4	12	18.78	63.11	17.38	12.86
7	5	3	4	12	18.82	63.16	17.42	12.91
8	5	3	4	12	18.76	63.08	17.4	12.88
9	5	3	4	12	18.78	63.05	17.35	12.97
10	5	3	4	12	18.77	63.09	17.35	12.85
11	5	3	4	12	18.76	63.08	17.36	12.77
12	5	3	4	12	18.7	63.03	17.41	12.78
13	5	3	4	12	18.82	63.08	17.33	12.94
14	5	3	4	12	18.8	63.05	17.33	12.88
15	5	3	4	12	18.8	63.04	17.39	12.79
16	5	3	4	12	18.77	63.11	17.43	12.97
17	5	3	4	12	18.82	63.05	17.32	13.02
18	5	3	4	12	18.82	63.03	17.33	12.98
19	5	3	4	12	18.75	63.04	17.43	12.76
20	5	3	4	12	18.83	63.2	17.41	12.96

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

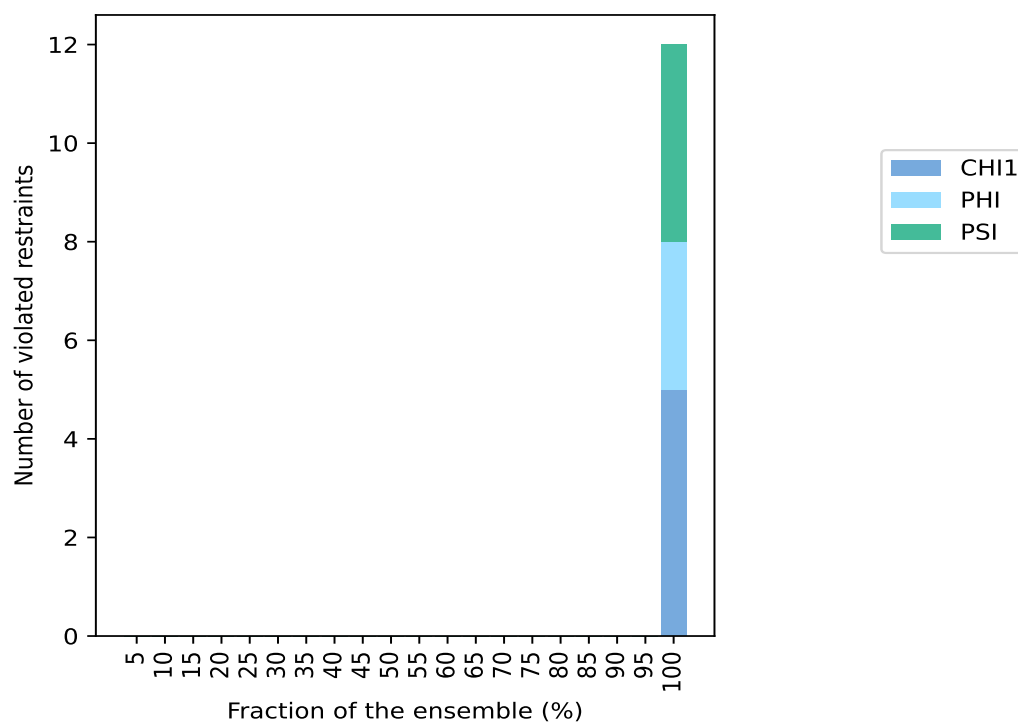
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Number of violated restraints				Fraction of the ensemble	
CHI1	PHI	PSI	Total	Count ¹	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
5	3	4	12	20	100.0

¹ Number of models with violations

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

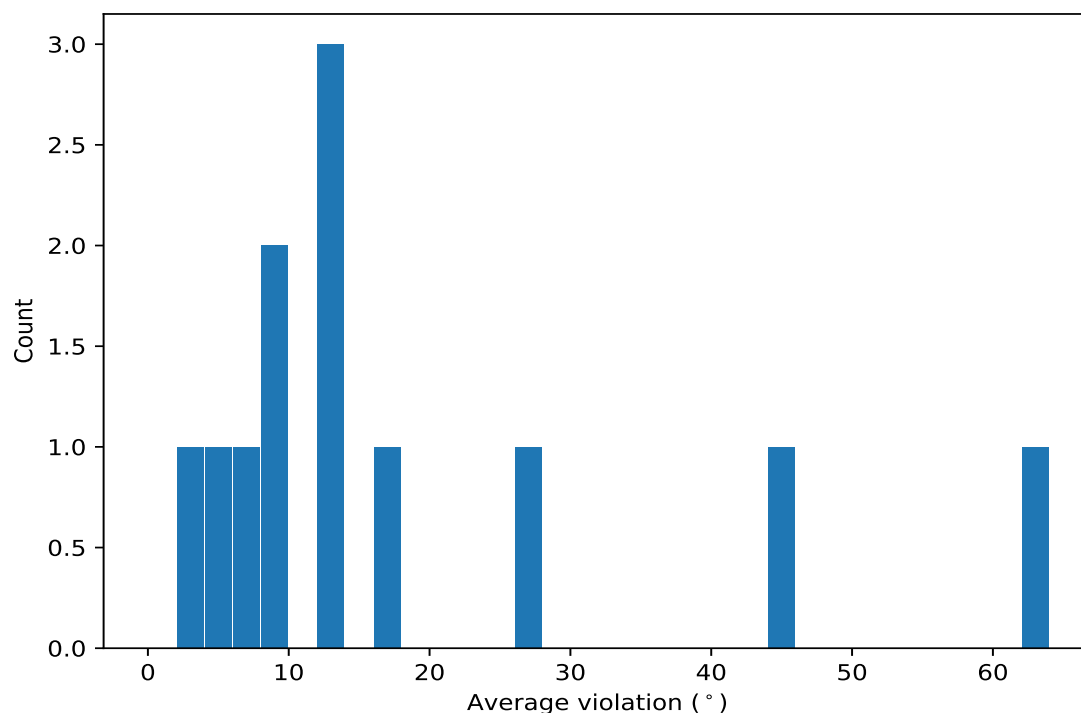


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

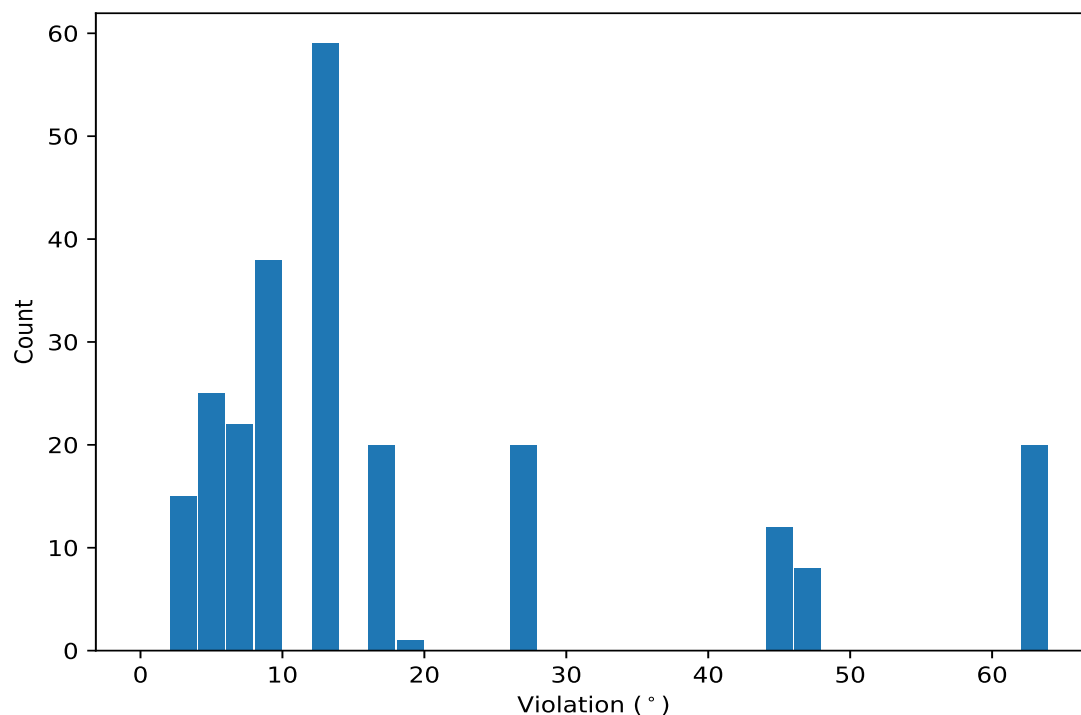
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	20	63.07	0.06	63.08
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	20	45.95	0.13	45.94
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	20	26.46	0.07	26.47
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	20	17.51	0.19	17.49
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	20	13.9	0.58	13.78
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	20	13.03	0.08	13.04
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	20	12.77	0.14	12.73
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	20	8.9	0.08	8.88
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	20	8.53	0.28	8.52
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	20	7.5	0.12	7.48
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	20	4.05	0.08	4.06
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	20	3.97	0.21	4.06

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 (°)
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	20	63.2
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	7	63.16
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	4	63.11
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	6	63.11
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	16	63.11
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	2	63.09
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	10	63.09
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	1	63.08
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	3	63.08
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	8	63.08
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	11	63.08
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	13	63.08
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	9	63.05
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	14	63.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	17	63.05
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	15	63.04
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	19	63.04
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	12	63.03
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	18	63.03
(1,16)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:CB	1:7:A:PHE:CG	5	62.86
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	16	46.15
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	7	46.14
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	2	46.12
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	19	46.11
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	15	46.09
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	20	46.07
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	8	46.05
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	1	46.02
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	3	45.97
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	6	45.94
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	12	45.94
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	4	45.89
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	18	45.88
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	11	45.86
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	17	45.86
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	13	45.82
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	14	45.82
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	9	45.81
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	10	45.77
(1,17)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:CB	1:8:A:PHE:CG	5	45.75
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	20	26.58
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	7	26.55
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	19	26.55
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	15	26.52
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	18	26.52
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	2	26.49
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	10	26.49
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	5	26.48
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	13	26.48
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	6	26.47
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	16	26.47
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	4	26.46
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	9	26.46
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	3	26.43
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	11	26.42
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	12	26.38
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	8	26.37
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	1	26.36
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	14	26.35
(1,13)	1:9:A:ARG:C	1:10:A:ASP:N	1:10:A:ASP:CA	1:10:A:ASP:C	17	26.33
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	5	18.21
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	15	17.71
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	2	17.63
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	3	17.62
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	19	17.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	10	17.57
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	14	17.54
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	17	17.52
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	12	17.51
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	9	17.5
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	6	17.48
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	7	17.43
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	20	17.42
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	8	17.41
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	18	17.41
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1	17.39
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	4	17.38
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	13	17.38
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	11	17.3
(1,3)	1:4:A:LEU:C	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	16	17.28
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	5	16.39
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	13	13.93
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	7	13.9
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	4	13.87
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	11	13.86
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	16	13.84
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	1	13.82
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	10	13.82
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	6	13.81
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	20	13.79
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	8	13.77
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	14	13.77
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	3	13.75
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	19	13.75
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	15	13.74
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	18	13.74
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	2	13.65
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	9	13.64
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	17	13.63
(1,14)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:CB	1:4:A:LEU:CG	12	13.61
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	16	13.17
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	2	13.16
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	1	13.11
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	7	13.1
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	20	13.07
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	13	13.06
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	14	13.06
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	4	13.05
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	18	13.05
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	12	13.04
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	17	13.04
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	8	13.03
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	9	13.03
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	3	13.01
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	10	13.01
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	17	13.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	6	13.0
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	15	12.97
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	19	12.96
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	2	12.95
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	4	12.95
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	9	12.91
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	18	12.91
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	5	12.9
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	5	12.86
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	20	12.85
(1,8)	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1:8:A:PHE:N	11	12.84
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	13	12.81
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	16	12.77
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	8	12.73
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	6	12.72
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	7	12.72
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	1	12.71
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	11	12.7
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	14	12.7
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	10	12.69
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	3	12.66
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	15	12.61
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	19	12.56
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:PHE:N	12	12.52
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	17	9.07
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	5	9.04
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	14	9.0
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	1	8.98
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	4	8.96
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	11	8.94
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	6	8.92
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	10	8.91
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	2	8.9
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	8	8.9
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	3	8.87
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	7	8.86
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	9	8.86
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	13	8.86
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	16	8.86
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	18	8.86
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	4	8.85
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	9	8.84
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	18	8.84
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	17	8.83
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	20	8.82
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	12	8.81
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	19	8.81
(1,7)	1:6:A:LYS:C	1:7:A:PHE:N	1:7:A:PHE:CA	1:7:A:PHE:C	15	8.78
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	2	8.77
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	20	8.77
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	13	8.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	5	8.73
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	12	8.57
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	8	8.53
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	14	8.52
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	6	8.48
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	11	8.45
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	19	8.44
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	16	8.42
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	15	8.38
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	7	8.3
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	1	8.25
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	10	7.93
(1,4)	1:5:A:SER:N	1:5:A:SER:CA	1:5:A:SER:C	1:6:A:LYS:N	3	7.85
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	5	7.84
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	14	7.71
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	10	7.63
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	3	7.58
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	11	7.55
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	6	7.54
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	20	7.54
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	7	7.5
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	18	7.5
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	15	7.49
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	8	7.47
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	4	7.45
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	13	7.45
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	19	7.45
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	16	7.42
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	12	7.41
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	1	7.4
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	9	7.35
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	2	7.34
(1,18)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:CB	1:9:A:ARG:CG	17	7.3
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	17	4.23
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	20	4.21
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	13	4.2
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	15	4.2
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	5	4.19
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	10	4.18
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	14	4.17
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	10	4.17
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	1	4.12
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	4	4.11
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	7	4.11
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	19	4.11
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	2	4.1
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	4	4.09
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	11	4.08
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	18	4.08
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	11	4.08
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	13	4.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	7	4.07
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	16	4.07
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	15	4.06
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	18	4.06
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	3	4.04
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	8	4.02
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	6	4.01
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	1	3.99
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	9	3.99
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	12	3.98
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	17	3.95
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	6	3.93
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	5	3.92
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	9	3.91
(1,12)	1:9:A:ARG:N	1:9:A:ARG:CA	1:9:A:ARG:C	1:10:A:ASP:N	14	3.91
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	3	3.9
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	2	3.81
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	8	3.81
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	16	3.69
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	20	3.68
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	19	3.6
(1,21)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:CB	1:15:A:ARG:CG	12	3.55