Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 04:10 PM EDT

PDB ID	:	2L9U
BMRB ID	:	17488
Title	:	Spatial structure of dimeric ErbB3 transmembrane domain
Authors	:	Mineev, K.S.; Arseniev, A.S.
Deposited on	:	2011-02-24

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

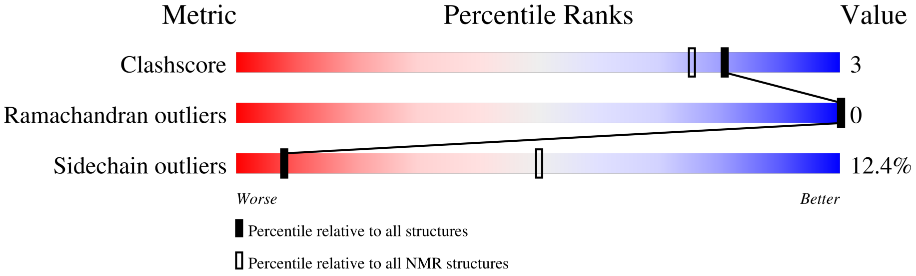
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 31%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	40	 25% 8% 68%
1	B	40	 55% 18% 28%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:654-A:666, B:640-B:668 (42)	0.11	6

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1320 atoms, of which 662 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total 660	C 213	H 331	N 67	O 45	S 4	0
1	B	40	Total 660	C 213	H 331	N 67	O 45	S 4	0

There are 18 discrepancies between the modelled and reference sequences:

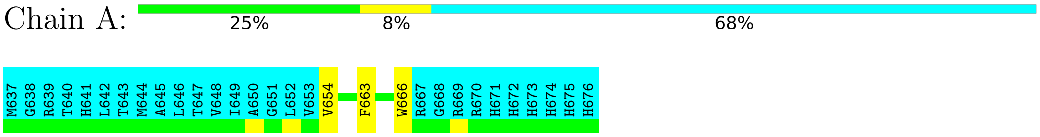
Chain	Residue	Modelled	Actual	Comment	Reference
A	637	MET	-	expression tag	UNP P21860
A	638	GLY	-	expression tag	UNP P21860
A	639	ARG	LYS	engineered mutation	UNP P21860
A	671	HIS	-	expression tag	UNP P21860
A	672	HIS	-	expression tag	UNP P21860
A	673	HIS	-	expression tag	UNP P21860
A	674	HIS	-	expression tag	UNP P21860
A	675	HIS	-	expression tag	UNP P21860
A	676	HIS	-	expression tag	UNP P21860
B	637	MET	-	expression tag	UNP P21860
B	638	GLY	-	expression tag	UNP P21860
B	639	ARG	LYS	engineered mutation	UNP P21860
B	671	HIS	-	expression tag	UNP P21860
B	672	HIS	-	expression tag	UNP P21860
B	673	HIS	-	expression tag	UNP P21860
B	674	HIS	-	expression tag	UNP P21860
B	675	HIS	-	expression tag	UNP P21860
B	676	HIS	-	expression tag	UNP P21860

4 Residue-property plots ⓘ

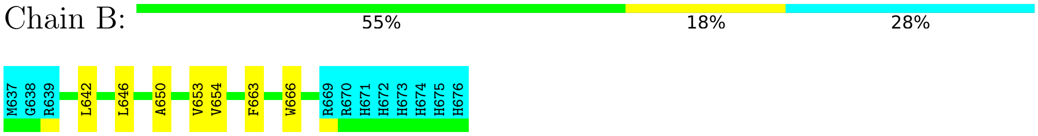
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Receptor tyrosine-protein kinase erbB-3



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

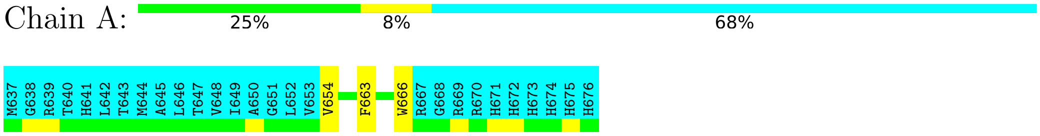


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

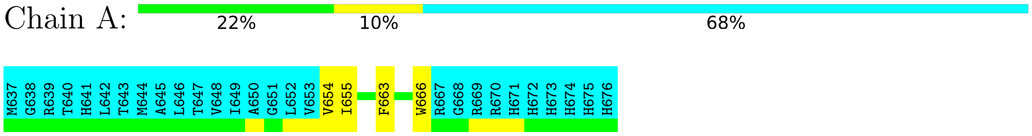


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

4.2.2 Score per residue for model 2

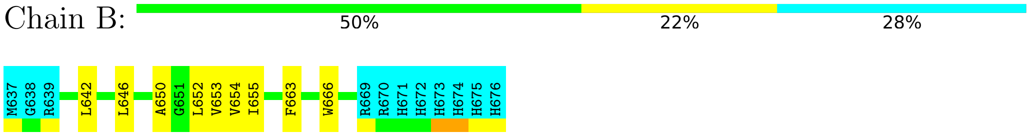
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

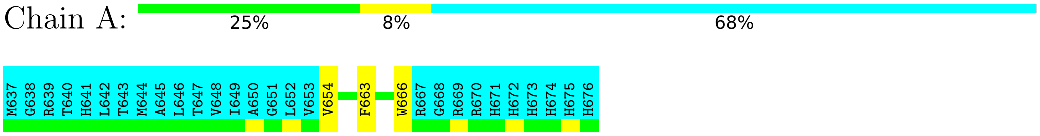
Chain B:



4.2.3 Score per residue for model 3

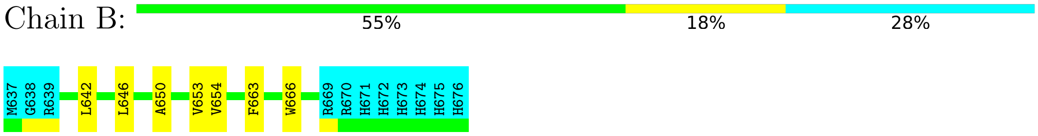
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

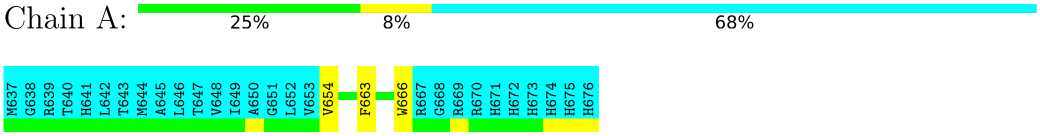
Chain B:



4.2.4 Score per residue for model 4

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



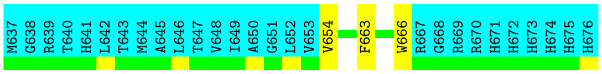
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.5 Score per residue for model 5

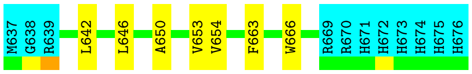
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:



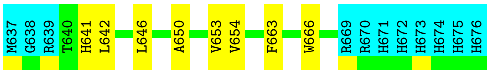
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

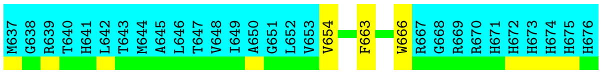
Chain B:



4.2.7 Score per residue for model 7

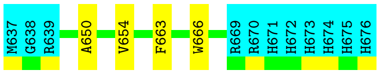
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

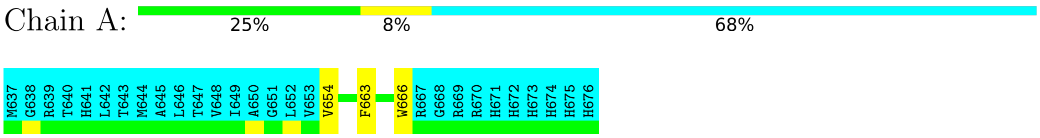
Chain B:



4.2.8 Score per residue for model 8

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



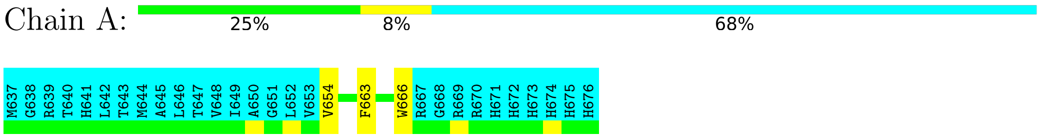
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.9 Score per residue for model 9

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



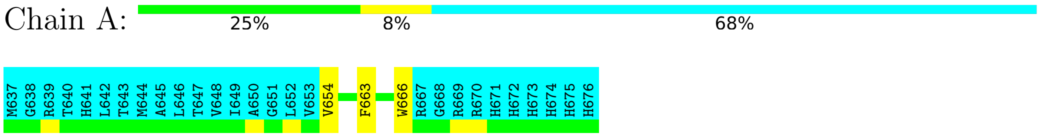
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.10 Score per residue for model 10

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:

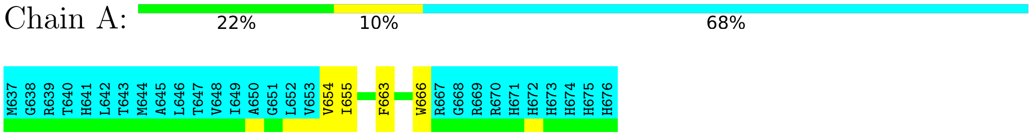


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

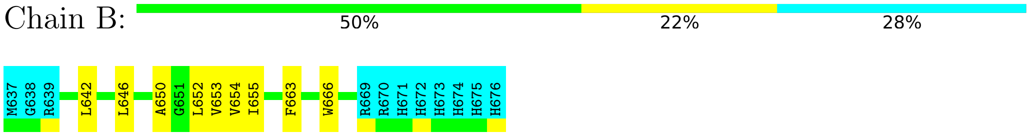
Chain B:

4.2.11 Score per residue for model 11

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

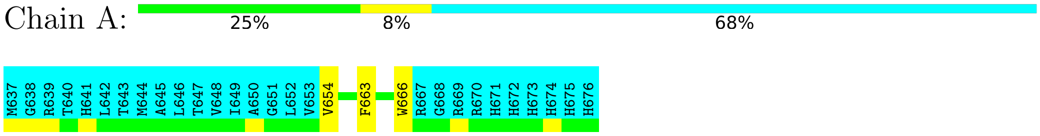


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

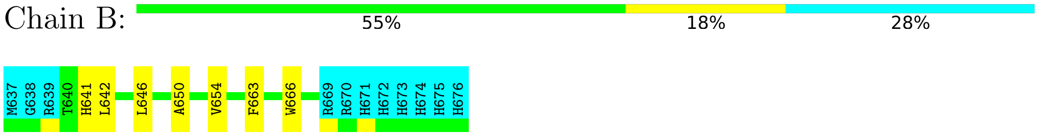


4.2.12 Score per residue for model 12

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

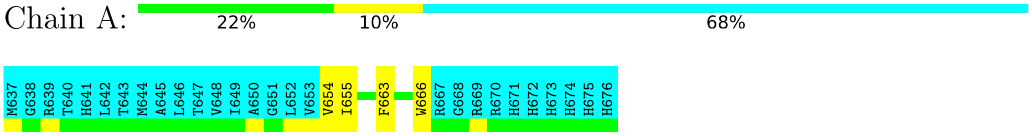


- Molecule 1: Receptor tyrosine-protein kinase erbB-3

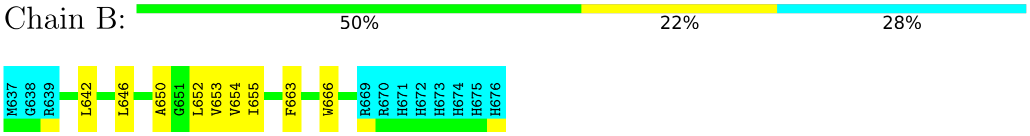


4.2.13 Score per residue for model 13

- Molecule 1: Receptor tyrosine-protein kinase erbB-3



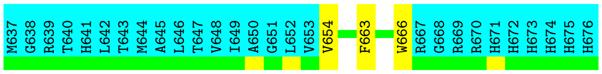
- Molecule 1: Receptor tyrosine-protein kinase erbB-3



4.2.14 Score per residue for model 14

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:

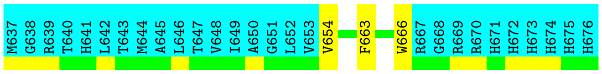
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:


4.2.15 Score per residue for model 15

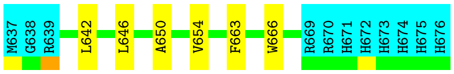
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

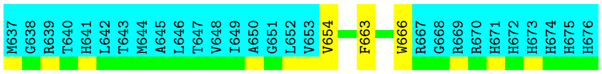
Chain B:

4.2.16 Score per residue for model 16

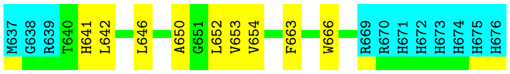
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

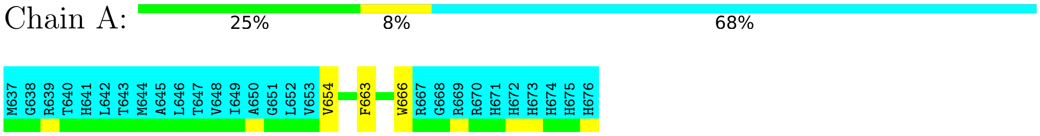
Chain B:

4.2.17 Score per residue for model 17

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



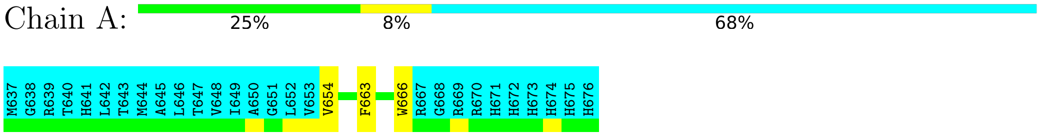
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.18 Score per residue for model 18

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



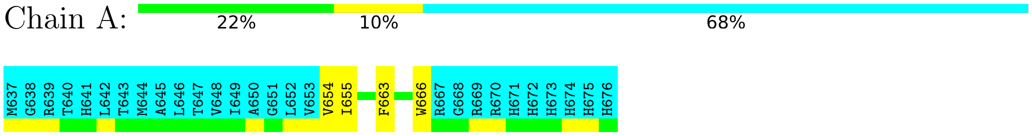
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.19 Score per residue for model 19

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



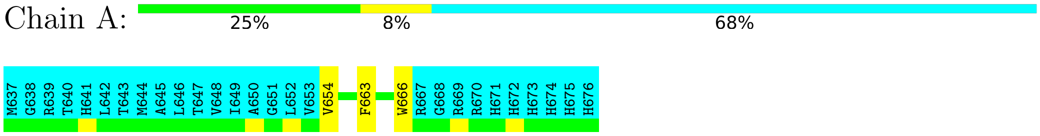
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:

4.2.20 Score per residue for model 20

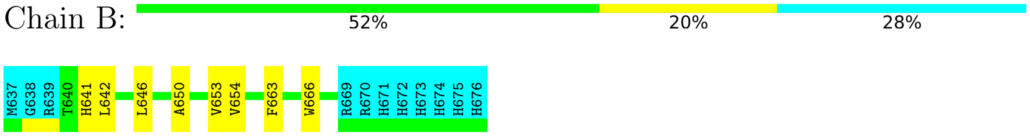
- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain A:



- Molecule 1: Receptor tyrosine-protein kinase erbB-3

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	**Classification**	**Version**
CYANA	refinement	3.0

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	526
Number of shifts mapped to atoms	526
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	31%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	110	110	110	0±0
1	B	224	238	238	2±1
All	All	6680	6960	6960	35

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:650:ALA:O	1:B:654:VAL:HG23	0.57	1.99	15	20
1:B:652:LEU:HA	1:B:655:ILE:HD12	0.52	1.81	11	4
1:B:642:LEU:O	1:B:646:LEU:HD12	0.41	2.15	15	11

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	13/40 (32%)	13±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	29/40 (72%)	28±0 (97±1%)	1±0 (3±1%)	0±0 (0±0%)	100	100
All	All	840/1600 (52%)	821 (98%)	19 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	11/33 (33%)	9±0 (82±0%)	2±0 (18±0%)	4	37
1	B	23/33 (70%)	21±0 (90±2%)	2±0 (10±2%)	12	58
All	All	680/1320 (52%)	596 (88%)	84 (12%)	8	50

All 5 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	663	PHE	20
1	A	666	TRP	20
1	B	663	PHE	20
1	B	666	TRP	20
1	B	641	HIS	4

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 31% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping (i)

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	526
Number of shifts mapped to atoms	526
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	**# values**	**Correction ± precision, *ppm***	**Suggested action**
$^{13}C_\alpha$	40	-0.84 ± 0.15	Should be checked
$^{13}C_\beta$	34	0.29 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	39	-0.10 ± 0.18	None needed (< 0.5 ppm)
^{15}N	40	0.35 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 31%, i.e. 186 atoms were assigned a chemical shift out of a possible 608. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	67/216 (31%)	28/90 (31%)	26/84 (31%)	13/42 (31%)
Sidechain	87/303 (29%)	60/208 (29%)	27/92 (29%)	0/3 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	32/89 (36%)	19/44 (43%)	12/42 (29%)	1/3 (33%)
Overall	186/608 (31%)	107/342 (31%)	65/218 (30%)	14/48 (29%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 521 atoms were assigned a chemical shift out of a possible 1186. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	202/410 (49%)	83/170 (49%)	79/160 (49%)	40/80 (50%)
Sidechain	275/596 (46%)	188/400 (47%)	81/172 (47%)	6/24 (25%)
Aromatic	44/180 (24%)	26/96 (27%)	17/68 (25%)	1/16 (6%)
Overall	521/1186 (44%)	297/666 (45%)	177/400 (44%)	47/120 (39%)

7.1.4 Statistically unusual chemical shifts ⓘ

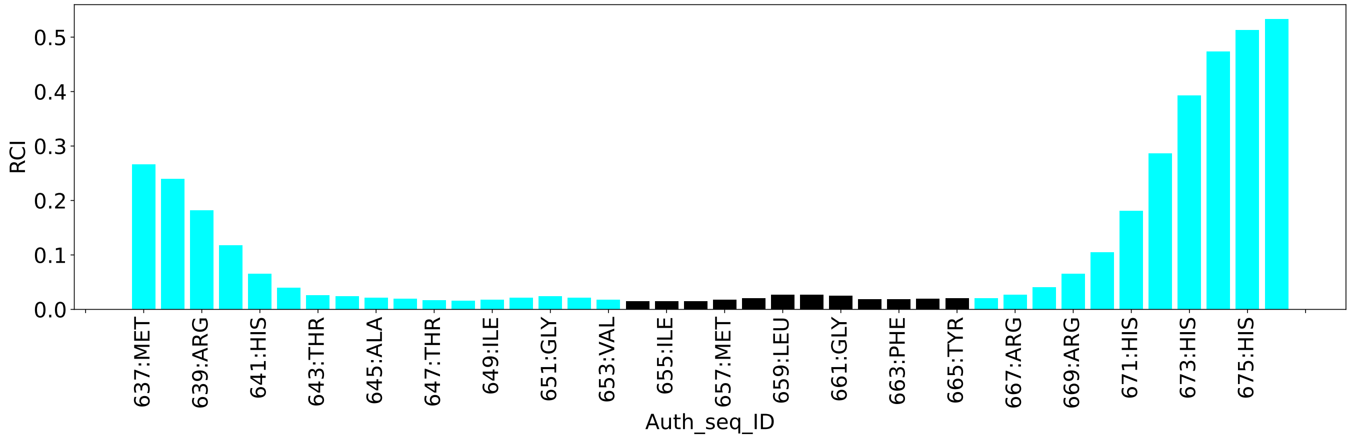
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	640	THR	HG1	4.65	0.08 – 2.19	16.6
1	A	647	THR	HG1	4.65	0.08 – 2.19	16.6
1	A	662	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	643	THR	HG1	4.64	0.08 – 2.19	16.6

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
637:MET
639:ARG
641:HIS
643:THR
645:ALA
647:THR
649:ILE
651:GLY
653:VAL
655:ILE
657:MET
659:LEU
661:GLY
663:PHE
665:TYR
667:ARG
669:ARG
671:HIS
673:HIS
675:HIS
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	891
Intra-residue (|i-j|=0)	444
Sequential (|i-j|=1)	236
Medium range (|i-j|>1 and |i-j|<5)	182
Long range (|i-j|≥5)	0
Inter-chain	29
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	8
Number of restraints per residue	11.1
Number of long range restraints per residue[1]	0.0

[1] Long 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 (i)

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 (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	22.4	0.2
0.2-0.5 (Medium)	6.2	0.49
>0.5 (Large)	6.4	2.66

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis

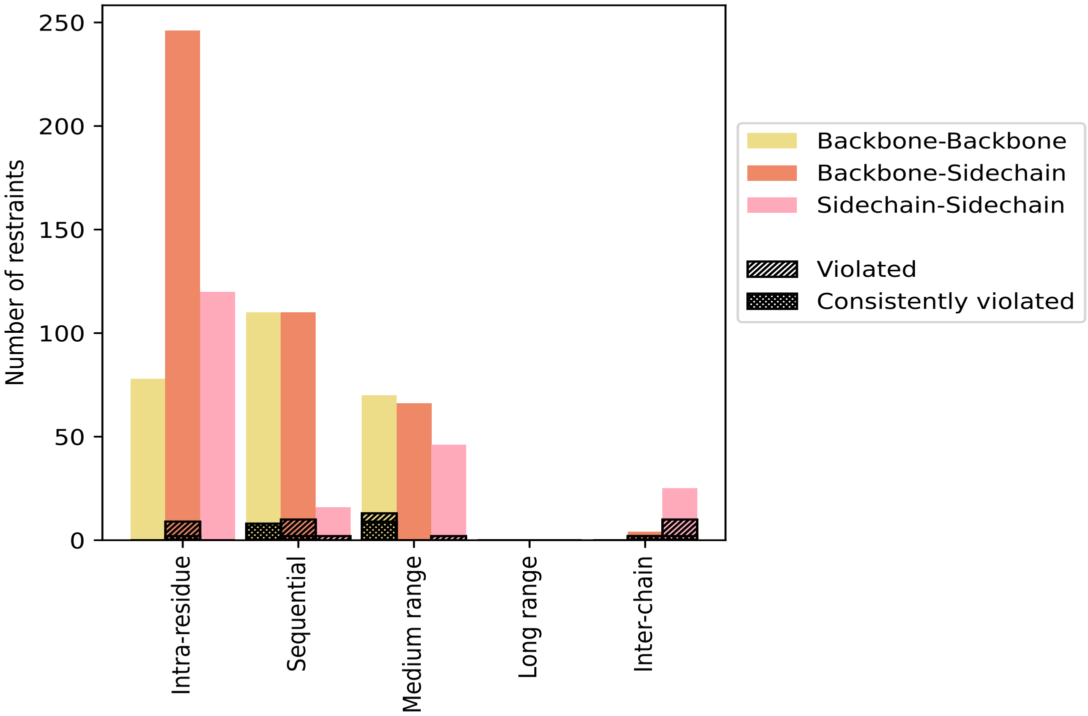
9.1 Summary of distance violations

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue ($\lvert i-j\rvert=0$)	444	49.8	9	2.0	1.0	2	0.5	0.2
Backbone-Backbone	78	8.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	246	27.6	9	3.7	1.0	2	0.8	0.2
Sidechain-Sidechain	120	13.5	0	0.0	0.0	0	0.0	0.0
Sequential ($\lvert i-j\rvert=1$)	236	26.5	20	8.5	2.2	10	4.2	1.1
Backbone-Backbone	110	12.3	8	7.3	0.9	8	7.3	0.9
Backbone-Sidechain	110	12.3	10	9.1	1.1	2	1.8	0.2
Sidechain-Sidechain	16	1.8	2	12.5	0.2	0	0.0	0.0
Medium range ($\lvert i-j\rvert>1$ & $\lvert i-j\rvert<5$)	182	20.4	15	8.2	1.7	9	4.9	1.0
Backbone-Backbone	70	7.9	13	18.6	1.5	9	12.9	1.0
Backbone-Sidechain	66	7.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	46	5.2	2	4.3	0.2	0	0.0	0.0
Long range ($\lvert i-j\rvert\geq5$)	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
Inter-chain	29	3.3	12	41.4	1.3	4	13.8	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.4	2	50.0	0.2	2	50.0	0.2
Sidechain-Sidechain	25	2.8	10	40.0	1.1	2	8.0	0.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	891	100.0	56	6.3	6.3	25	2.8	2.8
Backbone-Backbone	258	29.0	21	8.1	2.4	17	6.6	1.9
Backbone-Sidechain	426	47.8	21	4.9	2.4	6	1.4	0.7
Sidechain-Sidechain	207	23.2	14	6.8	1.6	2	1.0	0.2

[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 ⓘ



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 ⓘ

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	3	13	11	0	8	35	0.39	2.61	0.58	0.17
2	3	13	11	0	8	35	0.38	2.65	0.59	0.16
3	3	13	11	0	6	33	0.39	2.61	0.6	0.16
4	2	14	10	0	8	34	0.39	2.61	0.59	0.17
5	2	14	11	0	6	33	0.4	2.61	0.59	0.16
6	3	13	11	0	6	33	0.4	2.6	0.59	0.17
7	2	11	10	0	6	29	0.43	2.61	0.63	0.17
8	5	13	10	0	8	36	0.39	2.62	0.57	0.16
9	3	14	9	0	6	32	0.4	2.6	0.6	0.18
10	3	15	12	0	10	40	0.45	2.61	0.64	0.18
11	3	14	10	0	8	35	0.39	2.65	0.59	0.16

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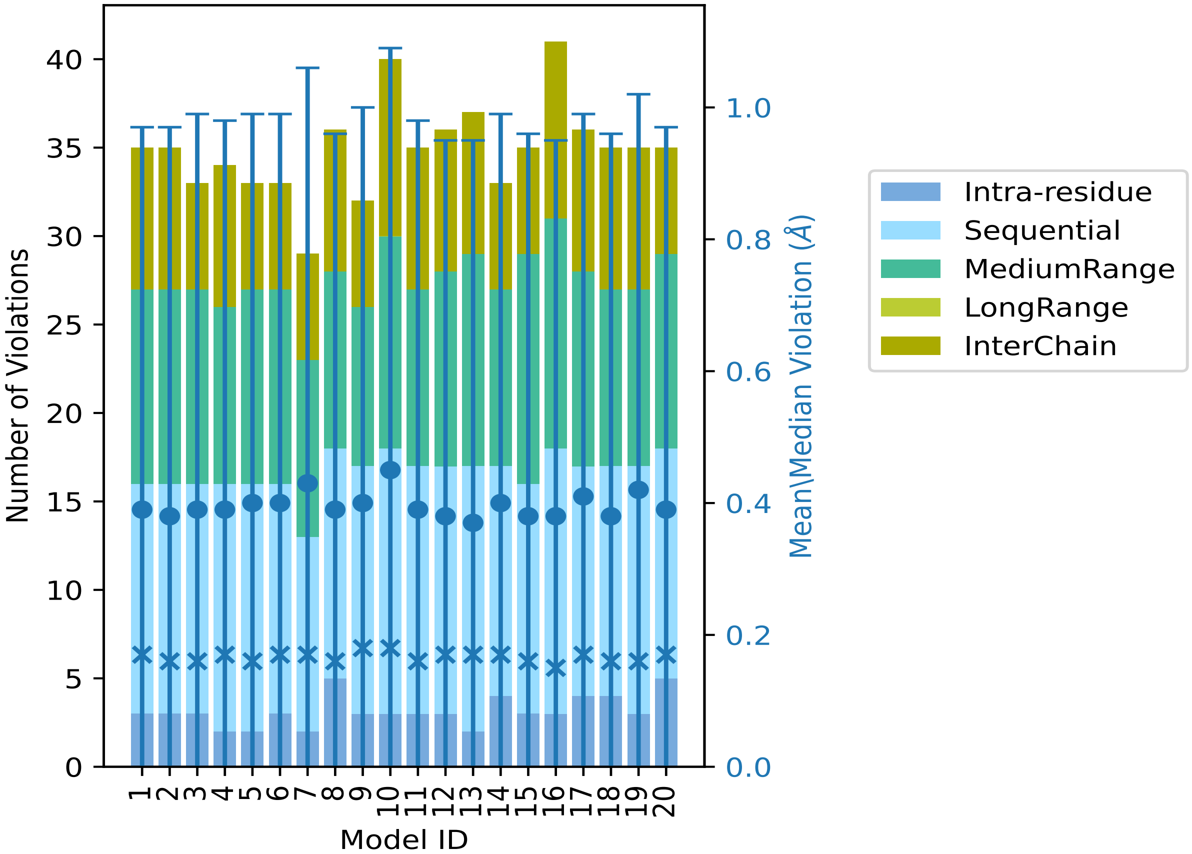
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	14	11	0	8	36	0.38	2.6	0.57	0.17
13	2	15	12	0	8	37	0.37	2.64	0.58	0.17
14	4	13	10	0	6	33	0.4	2.61	0.59	0.17
15	3	13	13	0	6	35	0.38	2.61	0.58	0.16
16	3	15	13	0	10	41	0.38	2.59	0.57	0.15
17	4	13	11	0	8	36	0.41	2.6	0.58	0.17
18	4	13	10	0	8	35	0.38	2.6	0.58	0.16
19	3	14	10	0	8	35	0.42	2.66	0.6	0.16
20	5	13	11	0	6	35	0.39	2.61	0.58	0.17

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

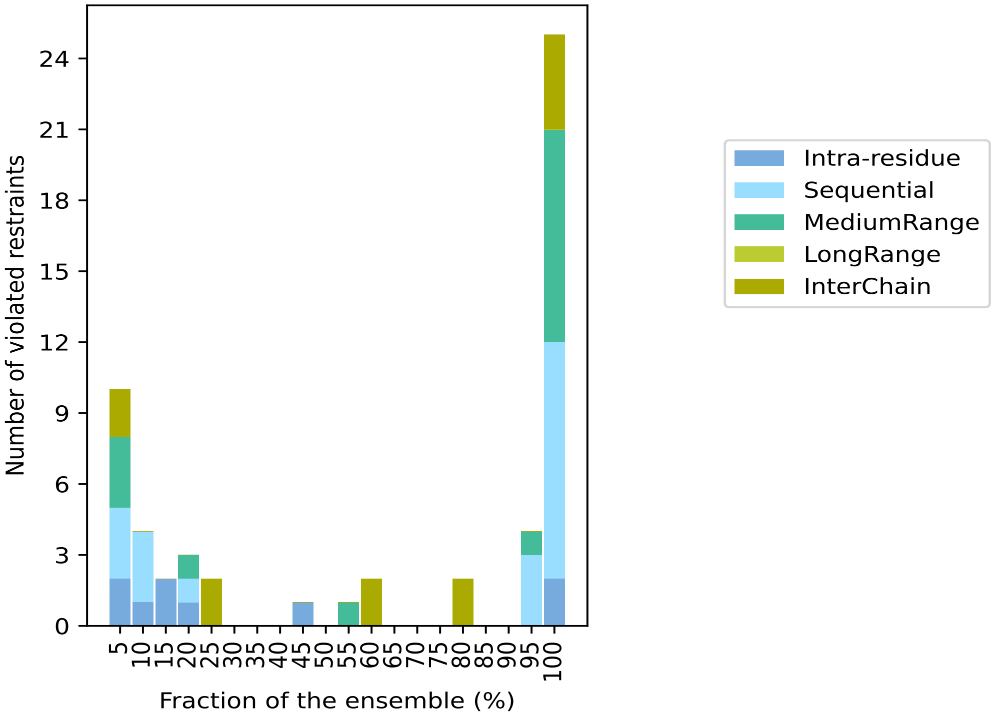
9.3 Distance violation statistics for the ensemble ⓘ

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, 835(IR:435, SQ:216, MR:167, LR:0, IC:17) 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]	%
2	3	3	0	2	10	1	5.0
1	3	0	0	0	4	2	10.0
2	0	0	0	0	2	3	15.0
1	1	1	0	0	3	4	20.0
0	0	0	0	2	2	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	2	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	2	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	3	1	0	0	4	19	95.0
2	10	9	0	4	25	20	100.0

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

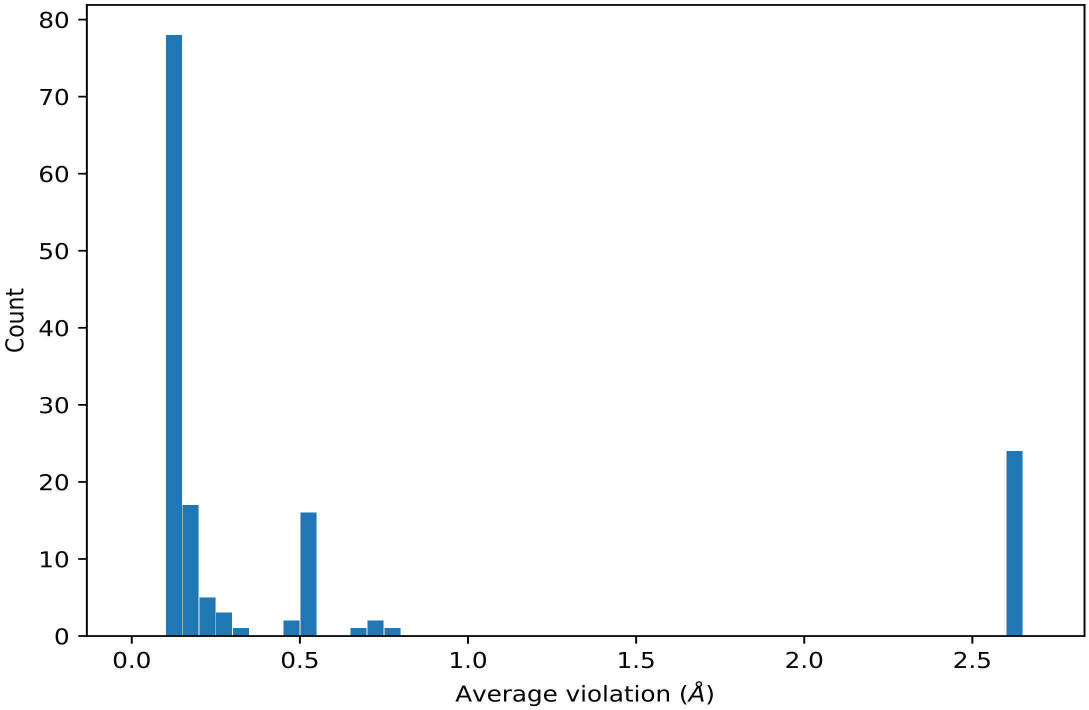
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	20	2.61	0.02	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	20	2.61	0.02	2.61

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	20	2.61	0.02	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	20	2.61	0.02	2.61
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	20	0.76	0.01	0.76
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	20	0.72	0.01	0.72
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	20	0.71	0.02	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	20	0.7	0.02	0.7
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	20	0.49	0.0	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	20	0.49	0.0	0.49
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	20	0.32	0.03	0.32
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	20	0.21	0.02	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	20	0.21	0.02	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	20	0.21	0.02	0.21
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	20	0.21	0.02	0.22
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	20	0.2	0.02	0.21
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	20	0.18	0.0	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	20	0.18	0.0	0.18
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	20	0.17	0.05	0.15
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	20	0.17	0.01	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	20	0.17	0.01	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	20	0.17	0.01	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	20	0.17	0.01	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	20	0.17	0.01	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	20	0.16	0.01	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	20	0.16	0.01	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	20	0.15	0.01	0.15
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	20	0.14	0.0	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	20	0.14	0.0	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	20	0.14	0.0	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	20	0.14	0.0	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	20	0.14	0.0	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	20	0.14	0.0	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	20	0.13	0.01	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	20	0.13	0.01	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	20	0.12	0.0	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	20	0.12	0.0	0.12
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	19	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	19	0.12	0.01	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	19	0.12	0.01	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	19	0.12	0.01	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	19	0.12	0.0	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	19	0.12	0.0	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	19	0.12	0.0	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	19	0.12	0.01	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	16	0.13	0.01	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	16	0.13	0.01	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	16	0.13	0.01	0.13
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	12	0.53	0.53	0.22
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	12	0.53	0.53	0.22
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	12	0.52	0.53	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	12	0.52	0.53	0.24
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	12	0.52	0.53	0.24
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	11	0.11	0.0	0.11
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	9	0.16	0.01	0.16
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	5	0.12	0.01	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	5	0.12	0.01	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	5	0.12	0.01	0.12
(1,411)	1:A:639:ARG:HB3	1:A:640:THR:H	4	0.3	0.09	0.35
(1,490)	1:B:671:HIS:H	1:B:671:HIS:HB3	4	0.19	0.0	0.19
(1,155)	1:A:662:THR:HG21	1:A:666:TRP:HE1	4	0.12	0.01	0.12
(1,155)	1:A:662:THR:HG22	1:A:666:TRP:HE1	4	0.12	0.01	0.12
(1,155)	1:A:662:THR:HG23	1:A:666:TRP:HE1	4	0.12	0.01	0.12
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG2	3	0.28	0.01	0.28
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG3	3	0.28	0.01	0.28
(1,59)	1:A:639:ARG:H	1:A:639:ARG:HB2	3	0.16	0.01	0.17
(1,285)	1:A:670:ARG:H	1:A:670:ARG:HB2	2	0.16	0.02	0.16
(1,343)	1:A:640:THR:HG21	1:A:641:HIS:H	2	0.16	0.01	0.16
(1,343)	1:A:640:THR:HG22	1:A:641:HIS:H	2	0.16	0.01	0.16

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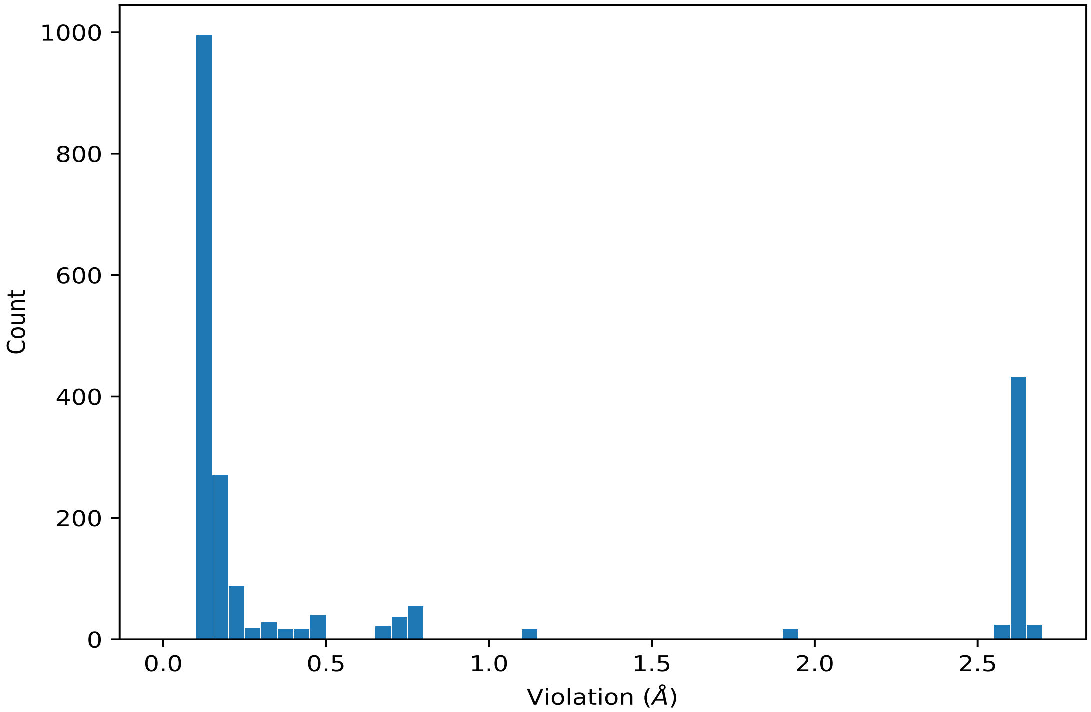
Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,343)	1:A:640:THR:HG23	1:A:641:HIS:H	2	0.16	0.01	0.16
(1,205)	1:A:665:TYR:HB2	1:A:666:TRP:H	2	0.12	0.01	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD21	2	0.12	0.0	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD22	2	0.12	0.0	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD23	2	0.12	0.0	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD21	2	0.12	0.0	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD22	2	0.12	0.0	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD23	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



9.5.2 Table : All distance violations ⓘ

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	19	2.66
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	19	2.66
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	19	2.66
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	19	2.66
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	19	2.66
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	19	2.66
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	19	2.66
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	19	2.66
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	19	2.66
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	19	2.66
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	19	2.66
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	19	2.66
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	19	2.66
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	19	2.66
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	19	2.66
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	19	2.66
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	19	2.66
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	19	2.66
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	19	2.66
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	19	2.66
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	19	2.66
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	19	2.66
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	19	2.66
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	19	2.66
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	2	2.65
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	2	2.65
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	2	2.65
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	2	2.65
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	2	2.65
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	2	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	2	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	2	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	2	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	2	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	2	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	2	2.65
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	11	2.65
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	11	2.65
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	11	2.65
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	11	2.65
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	11	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	11	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	11	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	11	2.65
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	11	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	11	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	11	2.65
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	11	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	2	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	2	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	2	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	2	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	2	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	2	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	2	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	2	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	2	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	2	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	2	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	2	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	11	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	11	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	11	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	11	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	11	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	11	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	11	2.65
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	11	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	11	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	11	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	11	2.65
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	11	2.65
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	13	2.64
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	13	2.64
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	13	2.64
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	13	2.64
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	13	2.64
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	13	2.64
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	13	2.64
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	13	2.64
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	13	2.64
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	13	2.64
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	13	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	13	2.64
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	13	2.63
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	13	2.63
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	13	2.63
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	13	2.63
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	13	2.63
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	13	2.63
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	13	2.63
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	13	2.63
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	13	2.63
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	13	2.63
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	13	2.63
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	13	2.63
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	8	2.62
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	8	2.62
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	8	2.62
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	8	2.62
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	8	2.62
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	8	2.62
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	8	2.62
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	8	2.62
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	8	2.62
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	8	2.62
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	8	2.62
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	8	2.62
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	8	2.62
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	8	2.62
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	8	2.62
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	8	2.62
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	8	2.62
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	8	2.62
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	8	2.62
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	8	2.62
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	8	2.62
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	8	2.62
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	8	2.62
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	8	2.62
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	3	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	3	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	3	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	3	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	3	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	3	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	3	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	3	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	3	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	3	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	3	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	3	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	5	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	5	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	5	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	5	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	5	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	5	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	5	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	5	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	5	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	5	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	5	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	5	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	7	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	7	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	7	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	7	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	7	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	7	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	7	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	7	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	7	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	7	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	7	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	7	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	10	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	10	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	10	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	10	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	10	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	10	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	10	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	10	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	10	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	10	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	10	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	10	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	14	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	14	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	14	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	14	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	14	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	14	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	14	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	14	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	14	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	14	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	14	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	14	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	15	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	15	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	15	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	15	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	15	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	15	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	15	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	15	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	15	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	15	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	15	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	15	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	20	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	20	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	20	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	20	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	20	2.61
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	20	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	20	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	20	2.61
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	20	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	20	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	20	2.61
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	20	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	1	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	1	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	1	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	1	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	1	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	1	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	1	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	1	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	1	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	1	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	1	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	1	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	4	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	4	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	4	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	4	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	4	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	4	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	4	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	4	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	4	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	4	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	4	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	4	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	5	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	5	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	5	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	5	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	5	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	5	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	5	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	5	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	5	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	5	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	5	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	5	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	7	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	7	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	7	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	7	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	7	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	7	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	7	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	7	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	7	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	7	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	7	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	7	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	10	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	10	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	10	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	10	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	10	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	10	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	10	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	10	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	10	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	10	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	10	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	10	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	14	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	14	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	14	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	14	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	14	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	14	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	14	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	14	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	14	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	14	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	14	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	14	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	15	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	15	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	15	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	15	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	15	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	15	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	15	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	15	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	15	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	15	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	15	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	15	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	20	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	20	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	20	2.61
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	20	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	20	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	20	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	20	2.61
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	20	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	20	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	20	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	20	2.61
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	20	2.61
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	1	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	1	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	1	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	1	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	1	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	1	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	1	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	1	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	1	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	1	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	1	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	1	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	4	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	4	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	4	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	4	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	4	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	4	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	4	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	4	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	4	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	4	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	4	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	4	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	6	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	6	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	6	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	6	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	6	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	6	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	6	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	6	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	6	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	6	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	6	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	6	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	9	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	9	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	9	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	9	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	9	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	9	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	9	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	9	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	9	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	9	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	9	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	9	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	12	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	12	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	12	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	12	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	12	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	12	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	12	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	12	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	12	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	12	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	12	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	12	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	17	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	17	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	17	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	17	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	17	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	17	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	17	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	17	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	17	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	17	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	17	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	17	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	18	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	18	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	18	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	18	2.6
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	18	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	18	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	18	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	18	2.6
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	18	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	18	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	18	2.6
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	18	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	3	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	3	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	3	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	3	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	3	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	3	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	3	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	3	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	3	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	3	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	3	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	3	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	6	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	6	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	6	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	6	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	6	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	6	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	6	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	6	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	6	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	6	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	6	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	6	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	9	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	9	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	9	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	9	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	9	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	9	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	9	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	9	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	9	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	9	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	9	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	9	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	12	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	12	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	12	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	12	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	12	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	12	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	12	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	12	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	12	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	12	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	12	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	12	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	17	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	17	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	17	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	17	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	17	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	17	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	17	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	17	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	17	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	17	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	17	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	17	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	18	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	18	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	18	2.6
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	18	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	18	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	18	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	18	2.6
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	18	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	18	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	18	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	18	2.6
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	18	2.6
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD11	16	2.59
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD12	16	2.59
(1,848)	1:A:656:PHE:HD1	1:B:652:LEU:HD13	16	2.59
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD11	16	2.59
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD12	16	2.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:656:PHE:HD2	1:B:652:LEU:HD13	16	2.59
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD11	16	2.59
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD12	16	2.59
(1,848)	1:A:656:PHE:HE1	1:B:652:LEU:HD13	16	2.59
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD11	16	2.59
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD12	16	2.59
(1,848)	1:A:656:PHE:HE2	1:B:652:LEU:HD13	16	2.59
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD1	16	2.59
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HD2	16	2.59
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE1	16	2.59
(1,847)	1:A:652:LEU:HD11	1:B:656:PHE:HE2	16	2.59
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD1	16	2.59
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HD2	16	2.59
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE1	16	2.59
(1,847)	1:A:652:LEU:HD12	1:B:656:PHE:HE2	16	2.59
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD1	16	2.59
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HD2	16	2.59
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE1	16	2.59
(1,847)	1:A:652:LEU:HD13	1:B:656:PHE:HE2	16	2.59
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	10	1.94
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	10	1.94
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	10	1.94
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	10	1.94
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	10	1.94
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	10	1.94
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	10	1.94
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	10	1.94
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	10	1.93
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	10	1.93
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	10	1.93
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	10	1.93
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	10	1.93
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	10	1.93
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	10	1.93
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	10	1.93
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	16	1.14
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	16	1.14
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	16	1.14
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	16	1.14
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	16	1.14
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	16	1.14
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	16	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	16	1.14
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	16	1.14
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	16	1.14
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	16	1.14
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	16	1.14
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	16	1.14
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	16	1.14
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	16	1.14
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	16	1.14
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	17	0.78
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	17	0.78
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	17	0.78
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	17	0.78
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	17	0.78
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	17	0.78
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	17	0.78
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	17	0.78
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	19	0.78
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	19	0.78
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	19	0.78
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	19	0.78
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	19	0.78
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	19	0.78
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	19	0.78
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	19	0.78
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	19	0.77
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	19	0.77
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	19	0.77
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	19	0.77
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	19	0.77
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	19	0.77
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	19	0.77
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	19	0.77
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	4	0.77
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	19	0.77
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	17	0.76
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	17	0.76
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	17	0.76
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	17	0.76
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	17	0.76
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	17	0.76
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	17	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	17	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	1	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	2	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	3	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	5	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	6	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	8	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	9	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	10	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	11	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	12	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	13	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	14	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	15	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	16	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	17	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	18	0.76
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	20	0.76
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	7	0.76
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	13	0.76
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	19	0.75
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	2	0.74
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	11	0.74
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	19	0.74
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	12	0.73
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	13	0.73
(1,350)	1:B:640:THR:HA	1:B:641:HIS:H	7	0.72
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	10	0.72
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	15	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	1	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	3	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	4	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	5	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	6	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	7	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	8	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	9	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	10	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	14	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	15	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	17	0.72
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	20	0.72
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	2	0.72
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	11	0.72
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	19	0.72
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	4	0.71
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	5	0.71
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	11	0.71
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	12	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	6	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	7	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	8	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	12	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	13	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	15	0.71
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	18	0.71
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	3	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	8	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	9	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	14	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	16	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	20	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	1	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	3	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	4	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	5	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	9	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	10	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	14	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	17	0.7
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	20	0.7
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	1	0.69
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	2	0.69
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	6	0.69
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	17	0.69
(1,349)	1:A:640:THR:HA	1:A:641:HIS:H	18	0.69
(1,2)	1:B:656:PHE:HA	1:B:659:LEU:H	16	0.67
(1,1)	1:A:656:PHE:HA	1:A:659:LEU:H	16	0.64
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	1	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	2	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	3	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	4	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	6	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	7	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	8	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	9	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	10	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	11	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	12	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	13	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	14	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	15	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	16	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	17	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	18	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	19	0.49
(1,108)	1:B:645:ALA:HA	1:B:646:LEU:H	20	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	1	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	2	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	3	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	4	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	5	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	6	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	7	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	8	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	9	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	10	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	11	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	12	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	13	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	14	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	15	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	16	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	17	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	18	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	19	0.49
(1,107)	1:A:645:ALA:HA	1:A:646:LEU:H	20	0.49
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	8	0.43
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	8	0.43
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	8	0.43
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	8	0.43
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	8	0.43
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	8	0.43
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	8	0.43
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	8	0.41
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	8	0.41
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	8	0.41
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	8	0.41
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	8	0.41
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	8	0.41
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	8	0.41
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	8	0.41
(1,864)	1:A:667:ARG:HD2	1:B:663:PHE:HD1	10	0.39
(1,864)	1:A:667:ARG:HD2	1:B:663:PHE:HD2	10	0.39
(1,864)	1:A:667:ARG:HD2	1:B:663:PHE:HE1	10	0.39
(1,864)	1:A:667:ARG:HD2	1:B:663:PHE:HE2	10	0.39
(1,864)	1:A:667:ARG:HD3	1:B:663:PHE:HD1	10	0.39
(1,864)	1:A:667:ARG:HD3	1:B:663:PHE:HD2	10	0.39
(1,864)	1:A:667:ARG:HD3	1:B:663:PHE:HE1	10	0.39
(1,864)	1:A:667:ARG:HD3	1:B:663:PHE:HE2	10	0.39
(1,865)	1:A:663:PHE:HD1	1:B:667:ARG:HD2	10	0.38
(1,865)	1:A:663:PHE:HD1	1:B:667:ARG:HD3	10	0.38
(1,865)	1:A:663:PHE:HD2	1:B:667:ARG:HD2	10	0.38
(1,865)	1:A:663:PHE:HD2	1:B:667:ARG:HD3	10	0.38
(1,865)	1:A:663:PHE:HE1	1:B:667:ARG:HD2	10	0.38
(1,865)	1:A:663:PHE:HE1	1:B:667:ARG:HD3	10	0.38
(1,865)	1:A:663:PHE:HE2	1:B:667:ARG:HD2	10	0.38
(1,865)	1:A:663:PHE:HE2	1:B:667:ARG:HD3	10	0.38
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	4	0.38
(1,411)	1:A:639:ARG:HB3	1:A:640:THR:H	5	0.35
(1,411)	1:A:639:ARG:HB3	1:A:640:THR:H	11	0.35
(1,411)	1:A:639:ARG:HB3	1:A:640:THR:H	12	0.35
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	14	0.34
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	19	0.34
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	1	0.33
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	1	0.33
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	1	0.33
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	1	0.33
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	1	0.33
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	1	0.33
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	1	0.33
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	1	0.33
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	1	0.33
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	2	0.33
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	9	0.33
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	18	0.33
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	3	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	5	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	6	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	10	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	11	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	15	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	17	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	20	0.32
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	12	0.31
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	16	0.31
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	13	0.3
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	7	0.3
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	13	0.3
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG2	20	0.29
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG3	20	0.29
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG2	14	0.28
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG3	14	0.28
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	1	0.27
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	1	0.27
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	1	0.27
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	1	0.27
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	1	0.27
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	1	0.27
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	1	0.27
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	1	0.27
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG2	8	0.26
(1,813)	1:A:639:ARG:HA	1:A:639:ARG:HG3	8	0.26
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	19	0.26
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	1	0.22
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	6	0.22
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	9	0.22
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	12	0.22
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	18	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	1	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	3	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	4	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	5	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	6	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	7	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	9	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	10	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	12	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	14	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	15	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	17	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	18	0.22
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	20	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	5	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	5	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	5	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	6	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	6	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	6	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	11	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	11	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	11	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	13	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	13	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	13	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	15	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	15	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	15	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	16	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	16	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	16	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	17	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	17	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	17	0.22
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	20	0.22
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	20	0.22
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	20	0.22
(1,619)	1:A:640:THR:HA	1:A:640:THR:HG21	17	0.21
(1,619)	1:A:640:THR:HA	1:A:640:THR:HG22	17	0.21
(1,619)	1:A:640:THR:HA	1:A:640:THR:HG23	17	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	3	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	4	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	5	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	7	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	8	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	10	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	15	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	17	0.21
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	20	0.21
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	14	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	1	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	1	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	1	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	2	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	2	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	2	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	3	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	3	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	3	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	8	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	8	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	8	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	9	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	9	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	9	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	10	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	10	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	10	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	12	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	12	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	12	0.21
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	18	0.21
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	18	0.21
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	18	0.21
(1,202)	1:B:640:THR:HA	1:B:642:LEU:H	7	0.21
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	16	0.2
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	14	0.2
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	14	0.2
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	14	0.2
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	4	0.19
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	1	0.19
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	4	0.19
(1,490)	1:B:671:HIS:H	1:B:671:HIS:HB3	6	0.19
(1,490)	1:B:671:HIS:H	1:B:671:HIS:HB3	9	0.19
(1,490)	1:B:671:HIS:H	1:B:671:HIS:HB3	18	0.19
(1,490)	1:B:671:HIS:H	1:B:671:HIS:HB3	20	0.19
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	13	0.19
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	13	0.19
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	19	0.19
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	19	0.19
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	19	0.19
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	9	0.19
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	9	0.19
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	9	0.19
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	9	0.19
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	1	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	2	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	3	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	5	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	6	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	7	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	8	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	9	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	10	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	11	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	12	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	13	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	14	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	15	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	16	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	17	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	18	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	19	0.18
(1,88)	1:B:659:LEU:HA	1:B:660:GLY:H	20	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	2	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	3	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	5	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	6	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	7	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	8	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	9	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	10	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	11	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	12	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	13	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	14	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	15	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	17	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	19	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	20	0.18
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	11	0.18
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	11	0.18
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	11	0.18
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	11	0.18
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	11	0.18
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	11	0.18
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	11	0.18
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	11	0.18
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	18	0.18
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	18	0.18
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	18	0.18
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	18	0.18
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	18	0.18
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	18	0.18
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	18	0.18
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	18	0.18
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	12	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	6	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	6	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	6	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	11	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	11	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	11	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	15	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	15	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	15	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	16	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	16	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	16	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	17	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	17	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	17	0.18
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	20	0.18
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	20	0.18
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	20	0.18
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	4	0.18
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	4	0.18
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	4	0.18
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	1	0.18
(1,285)	1:A:670:ARG:H	1:A:670:ARG:HB2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	2	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	2	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	4	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	4	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	13	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	13	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	16	0.18
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	16	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	4	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	4	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	13	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	13	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	16	0.18
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	16	0.18
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	4	0.18
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	10	0.18
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	15	0.18
(1,87)	1:A:659:LEU:HA	1:A:660:GLY:H	16	0.17
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	12	0.17
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	12	0.17
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	12	0.17
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	12	0.17
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	12	0.17
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	12	0.17
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	12	0.17
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	12	0.17
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	13	0.17
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	13	0.17
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	13	0.17
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	13	0.17
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	13	0.17
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	13	0.17
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	13	0.17
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	13	0.17
(1,59)	1:A:639:ARG:H	1:A:639:ARG:HB2	14	0.17
(1,59)	1:A:639:ARG:H	1:A:639:ARG:HB2	20	0.17
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	11	0.17
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	13	0.17
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	2	0.17
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	11	0.17
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	13	0.17
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	1	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	1	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	1	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	2	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	2	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	2	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	3	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	3	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	3	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	5	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	5	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	5	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	8	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	8	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	8	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	9	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	9	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	9	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	10	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	10	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	10	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	12	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	12	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	12	0.17
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	18	0.17
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	18	0.17
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	18	0.17
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	12	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	6	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	6	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	7	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	7	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	10	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	10	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	14	0.17
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	14	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	2	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	2	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	6	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	6	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	7	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	10	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	10	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	14	0.17
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	14	0.17
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	12	0.17
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	2	0.16
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	2	0.16
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	2	0.16
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	2	0.16
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	2	0.16
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	2	0.16
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	2	0.16
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	2	0.16
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH11	4	0.16
(1,867)	1:A:663:PHE:HD1	1:B:667:ARG:HH12	4	0.16
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH11	4	0.16
(1,867)	1:A:663:PHE:HD2	1:B:667:ARG:HH12	4	0.16
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH11	4	0.16
(1,867)	1:A:663:PHE:HE1	1:B:667:ARG:HH12	4	0.16
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH11	4	0.16
(1,867)	1:A:663:PHE:HE2	1:B:667:ARG:HH12	4	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	11	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	11	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	11	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	11	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	11	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	11	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	11	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	11	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	13	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	13	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	13	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	13	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	13	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	13	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	13	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	13	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	18	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	18	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	18	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	18	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	18	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	18	0.16
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	18	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	3	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	5	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	8	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	10	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	11	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	14	0.16
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	15	0.16
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	2	0.16
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	19	0.16
(1,435)	1:A:654:VAL:HA	1:A:657:MET:H	16	0.16
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	10	0.16
(1,343)	1:A:640:THR:HG21	1:A:641:HIS:H	7	0.16
(1,343)	1:A:640:THR:HG22	1:A:641:HIS:H	7	0.16
(1,343)	1:A:640:THR:HG23	1:A:641:HIS:H	7	0.16
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	14	0.16
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	14	0.16
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	14	0.16
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	19	0.16
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	19	0.16
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	19	0.16
(1,319)	1:A:643:THR:HG21	1:A:644:MET:H	7	0.16
(1,319)	1:A:643:THR:HG22	1:A:644:MET:H	7	0.16
(1,319)	1:A:643:THR:HG23	1:A:644:MET:H	7	0.16
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	3	0.16
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	17	0.16
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	18	0.16
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	19	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	1	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	1	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	11	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	11	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	12	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	12	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	15	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	15	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	18	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	18	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	19	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	20	0.16
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	20	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	11	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	11	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	20	0.16
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	20	0.16
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	5	0.16
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	11	0.16
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	14	0.16
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	4	0.15
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	4	0.15
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	4	0.15
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	4	0.15
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	4	0.15
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	4	0.15
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	4	0.15
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	4	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	1	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	2	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	6	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	7	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	12	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	18	0.15
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	20	0.15
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	8	0.15
(1,59)	1:A:639:ARG:H	1:A:639:ARG:HB2	8	0.15
(1,436)	1:B:654:VAL:HA	1:B:657:MET:H	16	0.15
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	5	0.15
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	6	0.15
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	13	0.15
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	15	0.15
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	19	0.15
(1,344)	1:B:640:THR:HG21	1:B:641:HIS:H	4	0.15
(1,344)	1:B:640:THR:HG22	1:B:641:HIS:H	4	0.15
(1,344)	1:B:640:THR:HG23	1:B:641:HIS:H	4	0.15
(1,343)	1:A:640:THR:HG21	1:A:641:HIS:H	19	0.15
(1,343)	1:A:640:THR:HG22	1:A:641:HIS:H	19	0.15
(1,343)	1:A:640:THR:HG23	1:A:641:HIS:H	19	0.15
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	11	0.15
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	16	0.15
(1,285)	1:A:670:ARG:H	1:A:670:ARG:HB2	8	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	3	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	5	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	5	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	8	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	8	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD1	17	0.15
(1,242)	1:B:665:TYR:H	1:B:665:TYR:HD2	17	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	1	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	1	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	3	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	3	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	5	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	5	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	8	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	8	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	12	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	12	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	15	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	15	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	17	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	17	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	18	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	18	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD1	19	0.15
(1,241)	1:A:665:TYR:H	1:A:665:TYR:HD2	19	0.15
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	8	0.14
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	8	0.14
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	8	0.14
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	8	0.14
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	8	0.14
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	8	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	8	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	8	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	8	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	8	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	8	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	8	0.14
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	18	0.14
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	18	0.14
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	18	0.14
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	18	0.14
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	18	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	18	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	18	0.14
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	18	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	18	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	18	0.14
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	18	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	8	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	8	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	8	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	8	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	8	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	8	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	8	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	8	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	8	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	8	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	8	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	8	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	18	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	18	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	18	0.14
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	18	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	18	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	18	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	18	0.14
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	18	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	18	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	18	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	18	0.14
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	18	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	1	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	1	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	1	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	3	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	3	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	3	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	4	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	4	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	4	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	5	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	5	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	6	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	6	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	6	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	8	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	8	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	8	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	10	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	10	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	10	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	11	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	11	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	11	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	12	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	12	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	12	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	13	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	13	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	13	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	15	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	15	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	15	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	16	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	16	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	16	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	17	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	17	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	17	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	20	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	20	0.14
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	20	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	1	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	1	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	1	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	2	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	2	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	2	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	3	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	3	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	3	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	4	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	4	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	5	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	5	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	5	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	6	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	6	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	6	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	7	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	7	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	7	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	8	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	8	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	8	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	9	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	9	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	9	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	10	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	10	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	10	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	11	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	11	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	11	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	12	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	12	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	12	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	14	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	14	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	14	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	15	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	15	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	15	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	16	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	16	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	16	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	17	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	17	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	17	0.14
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	20	0.14
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	20	0.14
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	20	0.14
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	4	0.14
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	17	0.14
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	19	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	3	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	5	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	11	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	14	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	15	0.14
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	20	0.14
(1,55)	1:A:639:ARG:H	1:A:639:ARG:HD2	15	0.14
(1,55)	1:A:639:ARG:H	1:A:639:ARG:HD3	15	0.14
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	3	0.14
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	8	0.14
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	9	0.14
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	11	0.14
(1,411)	1:A:639:ARG:HB3	1:A:640:THR:H	13	0.14
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	11	0.14
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	19	0.14
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	4	0.14
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	4	0.14
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	4	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	1	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	2	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	3	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	8	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	9	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	16	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	17	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	18	0.14
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	20	0.14
(1,155)	1:A:662:THR:HG21	1:A:666:TRP:HE1	10	0.14
(1,155)	1:A:662:THR:HG22	1:A:666:TRP:HE1	10	0.14
(1,155)	1:A:662:THR:HG23	1:A:666:TRP:HE1	10	0.14
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	2	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	2	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	2	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	2	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	2	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	2	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	2	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	2	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD1	12	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HD2	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE1	12	0.13
(1,866)	1:A:667:ARG:HH11	1:B:663:PHE:HE2	12	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD1	12	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HD2	12	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE1	12	0.13
(1,866)	1:A:667:ARG:HH12	1:B:663:PHE:HE2	12	0.13
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	16	0.13
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	16	0.13
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	16	0.13
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	16	0.13
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	16	0.13
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	16	0.13
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	16	0.13
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	16	0.13
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	16	0.13
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	16	0.13
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	16	0.13
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	16	0.13
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	16	0.13
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	16	0.13
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	16	0.13
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	16	0.13
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	16	0.13
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	16	0.13
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	16	0.13
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	16	0.13
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	16	0.13
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	16	0.13
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	16	0.13
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	16	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	1	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	1	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	1	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	1	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	1	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	1	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	1	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	1	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	1	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	1	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	1	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	3	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	3	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	3	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	3	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	3	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	3	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	3	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	3	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	3	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	3	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	3	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	3	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	5	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	5	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	5	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	5	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	5	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	5	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	5	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	5	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	5	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	5	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	5	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	5	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	6	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	6	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	6	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	6	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	6	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	6	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	6	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	6	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	6	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	6	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	6	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	6	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	7	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	7	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	7	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	7	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	7	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	7	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	7	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	7	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	7	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	7	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	7	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	9	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	9	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	9	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	9	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	9	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	9	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	9	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	9	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	9	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	9	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	9	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	9	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	10	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	10	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	10	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	10	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	10	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	10	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	10	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	10	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	10	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	10	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	10	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	10	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	12	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	12	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	12	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	12	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	12	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	12	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	12	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	12	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	12	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	12	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	12	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	14	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	14	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	14	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	14	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	14	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	14	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	14	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	14	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	14	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	14	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	14	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	14	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	15	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	15	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	15	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	15	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	15	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	15	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	15	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	15	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	15	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	15	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	15	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	15	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	20	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	20	0.13
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	20	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	20	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	20	0.13
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	20	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	20	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	20	0.13
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	20	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	20	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	20	0.13
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	20	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	1	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	1	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	1	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	1	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	1	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	1	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	1	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	1	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	1	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	1	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	1	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	3	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	3	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	3	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	3	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	3	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	3	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	3	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	3	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	3	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	3	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	3	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	3	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	4	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	4	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	4	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	4	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	4	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	4	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	4	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	4	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	4	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	4	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	4	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	4	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	5	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	5	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	5	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	5	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	5	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	5	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	5	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	5	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	5	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	5	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	5	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	6	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	6	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	6	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	6	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	6	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	6	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	6	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	6	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	6	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	6	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	6	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	6	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	7	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	7	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	7	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	7	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	7	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	7	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	7	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	7	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	7	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	7	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	7	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	7	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	9	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	9	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	9	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	9	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	9	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	9	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	9	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	9	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	9	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	9	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	9	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	9	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	10	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	10	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	10	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	10	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	10	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	10	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	10	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	10	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	10	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	10	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	10	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	12	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	12	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	12	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	12	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	12	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	12	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	12	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	12	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	12	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	12	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	12	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	12	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	14	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	14	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	14	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	14	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	14	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	14	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	14	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	14	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	14	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	14	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	14	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	14	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	15	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	15	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	15	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	15	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	15	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	15	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	15	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	15	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	15	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	15	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	15	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	20	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	20	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	20	0.13
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	20	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	20	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	20	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	20	0.13
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	20	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	20	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	20	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	20	0.13
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	20	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	2	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	2	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	2	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	7	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	7	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	7	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	9	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	9	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	9	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	14	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	14	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	14	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	18	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	18	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	18	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD11	19	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD12	19	0.13
(1,846)	1:A:656:PHE:HA	1:B:659:LEU:HD13	19	0.13
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	13	0.13
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	13	0.13
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	13	0.13
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	18	0.13
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	18	0.13
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	18	0.13
(1,845)	1:A:659:LEU:HD11	1:B:656:PHE:HA	19	0.13
(1,845)	1:A:659:LEU:HD12	1:B:656:PHE:HA	19	0.13
(1,845)	1:A:659:LEU:HD13	1:B:656:PHE:HA	19	0.13
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	13	0.13
(1,80)	1:B:656:PHE:HA	1:B:660:GLY:H	16	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	6	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	7	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	10	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	12	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	18	0.13
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	19	0.13
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	2	0.13
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	8	0.13
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	11	0.13
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	13	0.13
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	19	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	2	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	11	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	13	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	15	0.13
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	19	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	5	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	5	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	5	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	6	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	6	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	6	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	10	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	10	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	10	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	13	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	13	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	13	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	17	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	17	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	17	0.13
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	20	0.13
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	20	0.13
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	20	0.13
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	1	0.13
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	2	0.13
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	17	0.13
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	18	0.13
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	20	0.13
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	13	0.13
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	13	0.13
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	11	0.13
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	19	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	1	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	2	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	4	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	5	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	8	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	12	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	16	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	17	0.13
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	18	0.13
(1,320)	1:B:643:THR:HG21	1:B:644:MET:H	7	0.13
(1,320)	1:B:643:THR:HG22	1:B:644:MET:H	7	0.13
(1,320)	1:B:643:THR:HG23	1:B:644:MET:H	7	0.13
(1,286)	1:B:670:ARG:H	1:B:670:ARG:HB2	2	0.13
(1,205)	1:A:665:TYR:HB2	1:A:666:TRP:H	10	0.13
(1,201)	1:A:640:THR:HA	1:A:642:LEU:H	6	0.13
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	13	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	13	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	13	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	13	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	13	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	13	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	13	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	13	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	13	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	13	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	13	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	13	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	19	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	19	0.12
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	19	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	19	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	19	0.12
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	19	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	19	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	19	0.12
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	19	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	19	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	19	0.12
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	19	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	13	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	13	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	13	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	13	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	13	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	13	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	13	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	13	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	13	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	13	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	13	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	19	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	19	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	19	0.12
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	19	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	19	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	19	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	19	0.12
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	19	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	19	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	19	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	19	0.12
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	19	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	4	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	4	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	4	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	4	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	4	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	4	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	4	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	4	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	4	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	4	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	4	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	4	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	16	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	16	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	16	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	16	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	16	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	16	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	16	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	16	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	16	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	16	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	16	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD21	17	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD22	17	0.12
(1,850)	1:A:656:PHE:HD1	1:B:652:LEU:HD23	17	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD21	17	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD22	17	0.12
(1,850)	1:A:656:PHE:HD2	1:B:652:LEU:HD23	17	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD21	17	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD22	17	0.12
(1,850)	1:A:656:PHE:HE1	1:B:652:LEU:HD23	17	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD21	17	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD22	17	0.12
(1,850)	1:A:656:PHE:HE2	1:B:652:LEU:HD23	17	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	16	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	16	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	16	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	16	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	16	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	16	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	16	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	16	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	16	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	16	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	16	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	16	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD1	17	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HD2	17	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE1	17	0.12
(1,849)	1:A:652:LEU:HD21	1:B:656:PHE:HE2	17	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD1	17	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HD2	17	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE1	17	0.12
(1,849)	1:A:652:LEU:HD22	1:B:656:PHE:HE2	17	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD1	17	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HD2	17	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE1	17	0.12
(1,849)	1:A:652:LEU:HD23	1:B:656:PHE:HE2	17	0.12
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	4	0.12
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	9	0.12
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	17	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD21	16	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD22	16	0.12
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD23	16	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD21	16	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD22	16	0.12
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD23	16	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	1	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	3	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	4	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	5	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	6	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	7	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	9	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	10	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	12	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	14	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	15	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	16	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	17	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	18	0.12
(1,528)	1:B:653:VAL:HA	1:B:654:VAL:H	20	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	1	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	3	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	4	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	5	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	6	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	7	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	8	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	9	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	10	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	12	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	14	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	16	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	17	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	18	0.12
(1,527)	1:A:653:VAL:HA	1:A:654:VAL:H	20	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	1	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	1	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	2	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	2	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	2	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	3	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	3	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	3	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	8	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	8	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	8	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	9	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	9	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	9	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	11	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	11	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	11	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	12	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	12	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	12	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	14	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	14	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	14	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	15	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	15	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	15	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	16	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	16	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	16	0.12
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	18	0.12
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	18	0.12
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	18	0.12
(1,412)	1:B:639:ARG:HB3	1:B:640:THR:H	4	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	1	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	1	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	1	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	2	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	2	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	2	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	3	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	3	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	3	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	5	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	5	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	6	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	6	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	6	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	9	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	9	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	9	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	10	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	10	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	10	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	11	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	11	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	11	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	12	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	12	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	12	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	15	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	15	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	15	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	16	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	16	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	16	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	17	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	17	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	17	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	18	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	18	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	18	0.12
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	20	0.12
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	20	0.12
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	20	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	1	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	2	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	4	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	5	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	8	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	12	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	16	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	17	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	18	0.12
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	20	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	6	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	7	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	10	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	13	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	14	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	15	0.12
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	20	0.12
(1,206)	1:B:665:TYR:HB2	1:B:666:TRP:H	10	0.12
(1,155)	1:A:662:THR:HG21	1:A:666:TRP:HE1	15	0.12
(1,155)	1:A:662:THR:HG22	1:A:666:TRP:HE1	15	0.12
(1,155)	1:A:662:THR:HG23	1:A:666:TRP:HE1	15	0.12
(3,2)	1:B:652:LEU:HA	1:B:655:ILE:H	16	0.11
(3,1)	1:A:652:LEU:HA	1:A:655:ILE:H	16	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	2	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	2	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	2	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	2	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	2	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	2	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	2	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	2	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	2	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	2	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	2	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	2	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD11	11	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD12	11	0.11
(1,859)	1:A:656:PHE:HD1	1:B:655:ILE:HD13	11	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD11	11	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD12	11	0.11
(1,859)	1:A:656:PHE:HD2	1:B:655:ILE:HD13	11	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD11	11	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD12	11	0.11
(1,859)	1:A:656:PHE:HE1	1:B:655:ILE:HD13	11	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD11	11	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD12	11	0.11
(1,859)	1:A:656:PHE:HE2	1:B:655:ILE:HD13	11	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	2	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	2	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	2	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	2	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	2	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	2	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	2	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	2	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	2	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	2	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	2	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD1	11	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HD2	11	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE1	11	0.11
(1,858)	1:A:655:ILE:HD11	1:B:656:PHE:HE2	11	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD1	11	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HD2	11	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE1	11	0.11
(1,858)	1:A:655:ILE:HD12	1:B:656:PHE:HE2	11	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD1	11	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HD2	11	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE1	11	0.11
(1,858)	1:A:655:ILE:HD13	1:B:656:PHE:HE2	11	0.11
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	13	0.11
(1,79)	1:A:656:PHE:HA	1:A:660:GLY:H	16	0.11
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD21	13	0.11
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD22	13	0.11
(1,634)	1:B:663:PHE:HD1	1:B:664:LEU:HD23	13	0.11
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD21	13	0.11
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD22	13	0.11
(1,634)	1:B:663:PHE:HD2	1:B:664:LEU:HD23	13	0.11
(1,633)	1:A:663:PHE:HD1	1:A:664:LEU:HD21	16	0.11
(1,633)	1:A:663:PHE:HD1	1:A:664:LEU:HD22	16	0.11
(1,633)	1:A:663:PHE:HD1	1:A:664:LEU:HD23	16	0.11
(1,633)	1:A:663:PHE:HD2	1:A:664:LEU:HD21	16	0.11
(1,633)	1:A:663:PHE:HD2	1:A:664:LEU:HD22	16	0.11
(1,633)	1:A:663:PHE:HD2	1:A:664:LEU:HD23	16	0.11
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	4	0.11
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	4	0.11
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	4	0.11
(1,42)	1:B:642:LEU:HD11	1:B:643:THR:H	19	0.11
(1,42)	1:B:642:LEU:HD12	1:B:643:THR:H	19	0.11
(1,42)	1:B:642:LEU:HD13	1:B:643:THR:H	19	0.11
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	4	0.11
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	4	0.11
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	8	0.11
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	8	0.11
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	8	0.11
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	14	0.11
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	14	0.11
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	14	0.11
(1,41)	1:A:642:LEU:HD11	1:A:643:THR:H	19	0.11
(1,41)	1:A:642:LEU:HD12	1:A:643:THR:H	19	0.11
(1,41)	1:A:642:LEU:HD13	1:A:643:THR:H	19	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	3	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	6	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	7	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	10	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	13	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	14	0.11
(1,360)	1:B:658:MET:HA	1:B:661:GLY:H	15	0.11
(1,359)	1:A:658:MET:HA	1:A:661:GLY:H	9	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	1	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	3	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	5	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	6	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	10	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	12	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	13	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	15	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	16	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	17	0.11
(1,25)	1:A:641:HIS:HA	1:A:645:ALA:H	20	0.11
(1,205)	1:A:665:TYR:HB2	1:A:666:TRP:H	9	0.11
(1,156)	1:B:662:THR:HG21	1:B:666:TRP:HE1	15	0.11
(1,156)	1:B:662:THR:HG22	1:B:666:TRP:HE1	15	0.11
(1,156)	1:B:662:THR:HG23	1:B:666:TRP:HE1	15	0.11
(1,155)	1:A:662:THR:HG21	1:A:666:TRP:HE1	2	0.11
(1,155)	1:A:662:THR:HG22	1:A:666:TRP:HE1	2	0.11
(1,155)	1:A:662:THR:HG23	1:A:666:TRP:HE1	2	0.11
(1,155)	1:A:662:THR:HG21	1:A:666:TRP:HE1	13	0.11
(1,155)	1:A:662:THR:HG22	1:A:666:TRP:HE1	13	0.11
(1,155)	1:A:662:THR:HG23	1:A:666:TRP:HE1	13	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value