



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:04 PM UTC

PDB ID : 5V4C / pdb_00005v4c
BMRB ID : 30270
Title : Peptide 38136 modified from fragment 21-37 of Plasmodium falciparum Cell-Traversal Protein for Ookinetes and Sporozoites (CeITOS)
Authors : Bermudez, A.; Patarroyo, M.E.
Deposited on : 2017-03-09

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

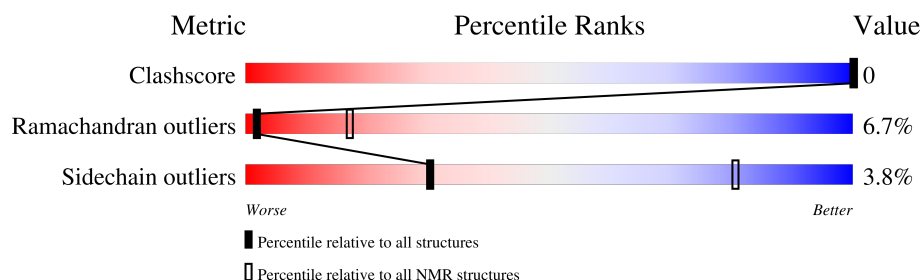
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	17	

2 Ensemble composition and analysis ⓘ

This entry contains 30 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 248 atoms, of which 120 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptide 38136.

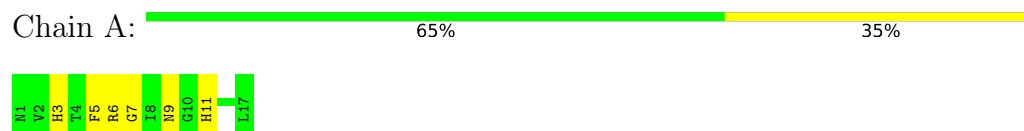
Mol	Chain	Residues	Atoms					Trace
1	A	17	Total	C	H	N	O	0
			248	76	120	27	25	

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: Peptide 38136

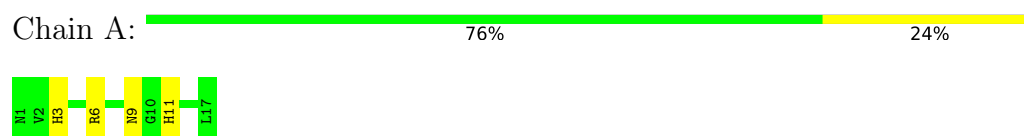


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

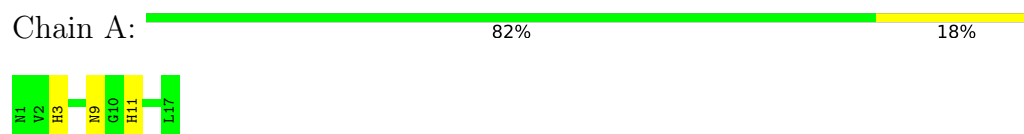
4.2.1 Score per residue for model 1

- Molecule 1: Peptide 38136



4.2.2 Score per residue for model 2

- Molecule 1: Peptide 38136



4.2.3 Score per residue for model 3

- Molecule 1: Peptide 38136

Chain A:  71% 24% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Peptide 38136

Chain A:  65% 29% 6%



4.2.5 Score per residue for model 5

- Molecule 1: Peptide 38136

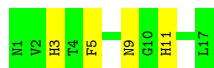
Chain A:  65% 24% 12%



4.2.6 Score per residue for model 6

- Molecule 1: Peptide 38136

Chain A:  76% 24%



4.2.7 Score per residue for model 7

- Molecule 1: Peptide 38136

Chain A:  71% 24% 6%



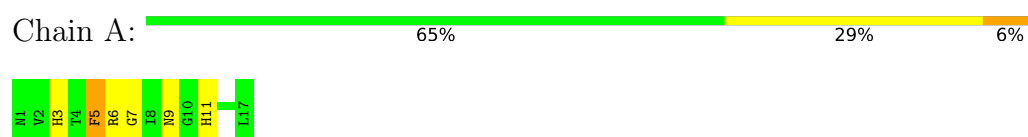
4.2.8 Score per residue for model 8

- Molecule 1: Peptide 38136



4.2.9 Score per residue for model 9

- Molecule 1: Peptide 38136



4.2.10 Score per residue for model 10

- Molecule 1: Peptide 38136



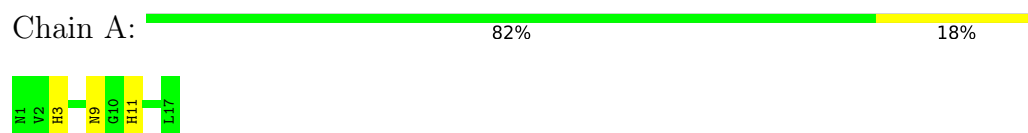
4.2.11 Score per residue for model 11

- Molecule 1: Peptide 38136



4.2.12 Score per residue for model 12

- Molecule 1: Peptide 38136



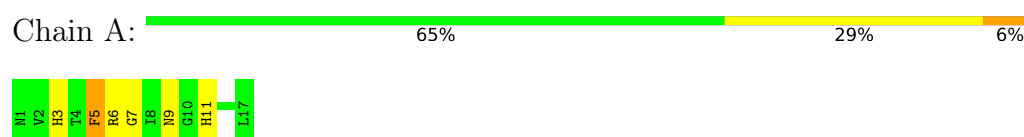
4.2.13 Score per residue for model 13

- Molecule 1: Peptide 38136



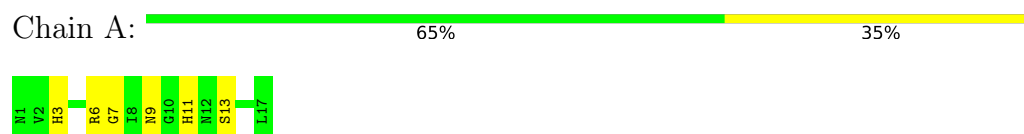
4.2.14 Score per residue for model 14

- Molecule 1: Peptide 38136



4.2.15 Score per residue for model 15

- Molecule 1: Peptide 38136



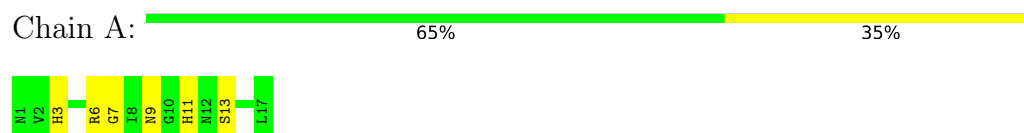
4.2.16 Score per residue for model 16

- Molecule 1: Peptide 38136



4.2.17 Score per residue for model 17

- Molecule 1: Peptide 38136



4.2.18 Score per residue for model 18

- Molecule 1: Peptide 38136

Chain A:  82% 18%



4.2.19 Score per residue for model 19

- Molecule 1: Peptide 38136

Chain A:  76% 24%



4.2.20 Score per residue for model 20

- Molecule 1: Peptide 38136

Chain A:  65% 29% 6%



4.2.21 Score per residue for model 21

- Molecule 1: Peptide 38136

Chain A:  76% 24%



4.2.22 Score per residue for model 22

- Molecule 1: Peptide 38136

Chain A:  65% 29% 6%



4.2.23 Score per residue for model 23

- Molecule 1: Peptide 38136



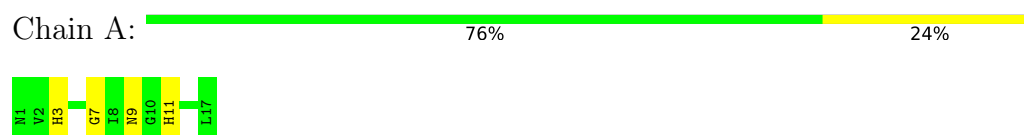
4.2.24 Score per residue for model 24

- Molecule 1: Peptide 38136



4.2.25 Score per residue for model 25

- Molecule 1: Peptide 38136



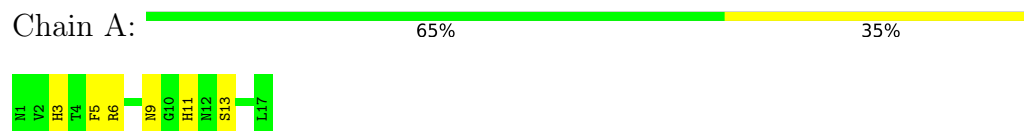
4.2.26 Score per residue for model 26

- Molecule 1: Peptide 38136



4.2.27 Score per residue for model 27

- Molecule 1: Peptide 38136



4.2.28 Score per residue for model 28

- Molecule 1: Peptide 38136

Chain A:  65% 29% 6%



4.2.29 Score per residue for model 29

- Molecule 1: Peptide 38136

Chain A:  82% 18%



4.2.30 Score per residue for model 30

- Molecule 1: Peptide 38136

Chain A:  65% 35%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 30 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Insight II	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	97
Number of shifts mapped to atoms	97
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.79±0.03	2±0/130 (1.7± 0.3%)	2.63±0.16	10±1/174 (5.8± 0.7%)
All	All	1.79	67/3900 (1.7%)	2.64	303/5220 (5.8%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.4
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	HIS	ND1-CE1	5.63	1.38	1.32	4	30
1	A	3	HIS	ND1-CE1	5.54	1.38	1.32	16	30
1	A	11	HIS	CE1-NE2	5.16	1.37	1.32	27	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	SER	CB-CA-C	16.21	134.74	111.73	10	3
1	A	3	HIS	ND1-CE1-NE2	12.00	120.40	108.40	6	30
1	A	11	HIS	ND1-CE1-NE2	11.79	120.19	108.40	20	30
1	A	11	HIS	CE1-NE2-CD2	-9.76	99.24	109.00	28	30
1	A	3	HIS	CE1-NE2-CD2	-9.34	99.66	109.00	6	30
1	A	5	PHE	CA-CB-CG	8.91	122.72	113.80	22	14
1	A	13	SER	CA-C-N	8.21	137.22	121.54	24	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	SER	C-N-CA	8.21	137.22	121.54	24	3
1	A	11	HIS	CA-CB-CG	7.42	121.22	113.80	26	1
1	A	15	SER	N-CA-CB	-7.24	101.20	112.13	24	3
1	A	11	HIS	CB-CG-CD2	-6.99	122.11	131.20	4	29
1	A	1	ASN	CA-CB-CG	6.96	119.56	112.60	16	1
1	A	11	HIS	CG-ND1-CE1	-6.37	98.47	109.30	21	30
1	A	12	ASN	CA-CB-CG	6.32	118.92	112.60	11	1
1	A	3	HIS	CG-ND1-CE1	-6.22	98.73	109.30	15	30
1	A	5	PHE	N-CA-C	6.12	120.33	112.86	16	1
1	A	4	THR	CA-CB-CG2	5.76	120.30	110.50	23	1
1	A	6	ARG	NE-CZ-NH2	5.43	124.09	119.20	4	15
1	A	9	ASN	CA-CB-CG	5.39	117.99	112.60	5	29
1	A	3	HIS	CB-CG-CD2	-5.17	124.48	131.20	30	11
1	A	11	HIS	ND1-CG-CD2	5.14	111.24	106.10	28	7
1	A	3	HIS	N-CA-C	5.04	116.47	111.07	29	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	5	PHE	Sidechain	8

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
All	All	3840	3600	3600	-

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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	15/17 (88%)	11±2 (72±10%)	3±1 (17±6%)	1±1 (6±4%)	2	18
All	All	431/510 (85%)	325 (75%)	77 (18%)	29 (7%)	2	17

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	GLY	18
1	A	5	PHE	7
1	A	14	SER	3
1	A	2	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	15/15 (100%)	14±1 (96±5%)	1±1 (4±5%)	30	81
All	All	450/450 (100%)	433 (96%)	17 (4%)	30	81

All 4 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	13	SER	8
1	A	6	ARG	7
1	A	5	PHE	1
1	A	4	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: 38135.txt

7.1.1 Bookkeeping

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

Total number of shifts	97
Number of shifts mapped to atoms	97
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 95 atoms were assigned a chemical shift out of a possible 213. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	35/87 (40%)	35/36 (97%)	0/34 (0%)	0/17 (0%)
Sidechain	53/102 (52%)	53/66 (80%)	0/30 (0%)	0/6 (0%)
Aromatic	7/24 (29%)	7/13 (54%)	0/9 (0%)	0/2 (0%)
Overall	95/213 (45%)	95/115 (83%)	0/73 (0%)	0/25 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 95 atoms were assigned a chemical shift out of a possible 213. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	35/87 (40%)	35/36 (97%)	0/34 (0%)	0/17 (0%)
Sidechain	53/102 (52%)	53/66 (80%)	0/30 (0%)	0/6 (0%)
Aromatic	7/24 (29%)	7/13 (54%)	0/9 (0%)	0/2 (0%)
Overall	95/213 (45%)	95/115 (83%)	0/73 (0%)	0/25 (0%)

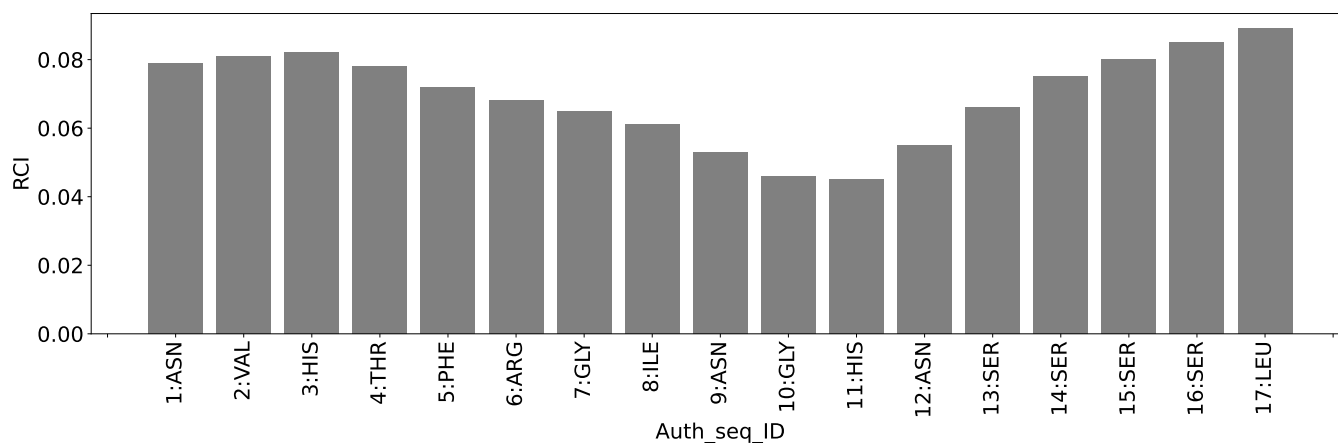
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	143
Intra-residue ($ i-j =0$)	78
Sequential ($ i-j =1$)	40
Medium range ($ i-j >1$ and $ i-j <5$)	23
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	16
Number of unmapped restraints	0
Number of restraints per residue	9.4
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	11.8	0.2
0.2-0.5 (Medium)	14.6	0.5
>0.5 (Large)	28.7	8.24

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.7	4.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

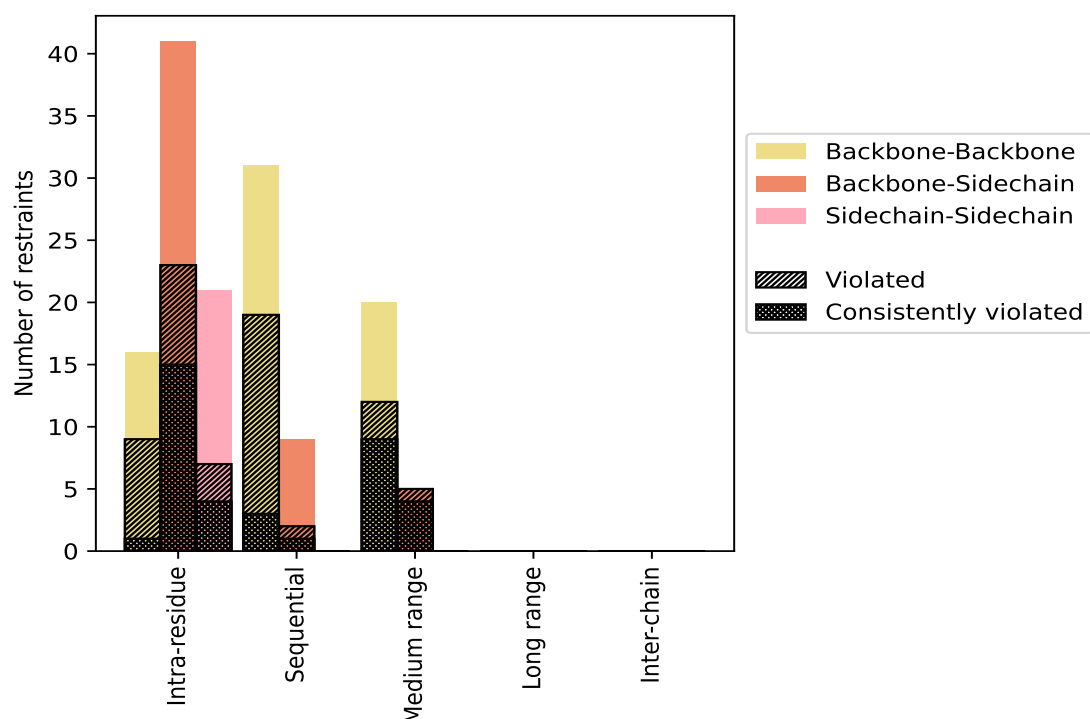
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	78	54.5	39	50.0	27.3	20	25.6	14.0
Backbone-Backbone	16	11.2	9	56.2	6.3	1	6.2	0.7
Backbone-Sidechain	41	28.7	23	56.1	16.1	15	36.6	10.5
Sidechain-Sidechain	21	14.7	7	33.3	4.9	4	19.0	2.8
Sequential (i-j =1)	40	28.0	21	52.5	14.7	4	10.0	2.8
Backbone-Backbone	31	21.7	19	61.3	13.3	3	9.7	2.1
Backbone-Sidechain	9	6.3	2	22.2	1.4	1	11.1	0.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	23	16.1	15	65.2	10.5	11	47.8	7.7
Backbone-Backbone	20	14.0	12	60.0	8.4	9	45.0	6.3
Backbone-Sidechain	3	2.1	3	100.0	2.1	2	66.7	1.4
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	2	1.4	2	100.0	1.4	2	100.0	1.4
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	143	100.0	77	53.8	53.8	37	25.9	25.9
Backbone-Backbone	67	46.9	40	59.7	28.0	13	19.4	9.1
Backbone-Sidechain	55	38.5	30	54.5	21.0	20	36.4	14.0
Sidechain-Sidechain	21	14.7	7	33.3	4.9	4	19.0	2.8

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	30	11	16	0	0	57	1.03	6.16	1.31	0.58
2	29	11	15	0	0	55	1.02	5.28	1.22	0.56
3	30	12	15	0	0	57	0.99	7.92	1.4	0.47
4	30	12	16	0	0	58	1.02	7.94	1.41	0.49
5	29	14	16	0	0	59	1.0	7.84	1.42	0.45
6	31	11	16	0	0	58	1.12	7.31	1.49	0.55
7	30	15	15	0	0	60	0.96	6.41	1.26	0.47
8	27	12	16	0	0	55	1.08	7.66	1.39	0.59
9	29	11	15	0	0	55	1.04	8.24	1.45	0.53
10	26	15	16	0	0	57	1.08	5.99	1.36	0.56

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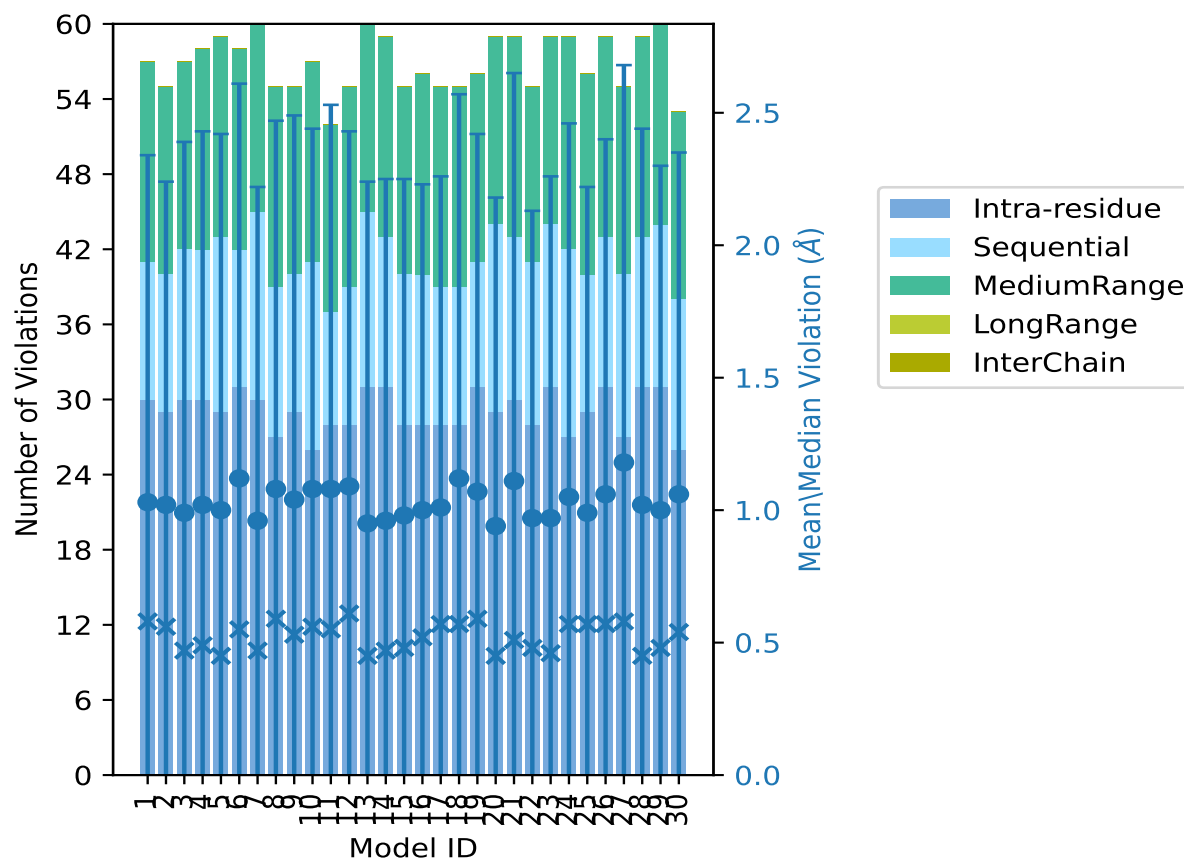
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	28	9	15	0	0	52	1.08	8.04	1.45	0.55
12	28	11	16	0	0	55	1.09	6.13	1.34	0.61
13	31	14	15	0	0	60	0.95	7.08	1.29	0.45
14	31	12	16	0	0	59	0.96	6.8	1.29	0.47
15	28	12	15	0	0	55	0.98	6.35	1.27	0.48
16	28	12	16	0	0	56	1.0	5.88	1.23	0.52
17	28	11	16	0	0	55	1.01	6.17	1.25	0.57
18	28	11	16	0	0	55	1.12	6.75	1.45	0.57
19	31	10	15	0	0	56	1.07	6.01	1.35	0.59
20	29	15	15	0	0	59	0.94	6.47	1.24	0.45
21	30	13	16	0	0	59	1.11	7.82	1.54	0.51
22	28	13	14	0	0	55	0.97	5.57	1.16	0.48
23	31	13	15	0	0	59	0.97	6.96	1.29	0.46
24	27	15	17	0	0	59	1.05	7.61	1.41	0.57
25	29	11	16	0	0	56	0.99	6.2	1.23	0.57
26	31	12	16	0	0	59	1.06	6.14	1.34	0.57
27	27	13	15	0	0	55	1.18	7.11	1.5	0.58
28	31	12	16	0	0	59	1.02	7.94	1.42	0.45
29	31	13	16	0	0	60	1.0	6.08	1.3	0.48
30	26	12	15	0	0	53	1.06	6.26	1.29	0.54

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 66(IR:39, SQ:19, MR:8, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	0	0	0	0	5	1	3.3
0	0	1	0	0	1	2	6.7
1	5	0	0	0	6	3	10.0
0	0	0	0	0	0	4	13.3
0	0	0	0	0	0	5	16.7
0	0	0	0	0	0	6	20.0

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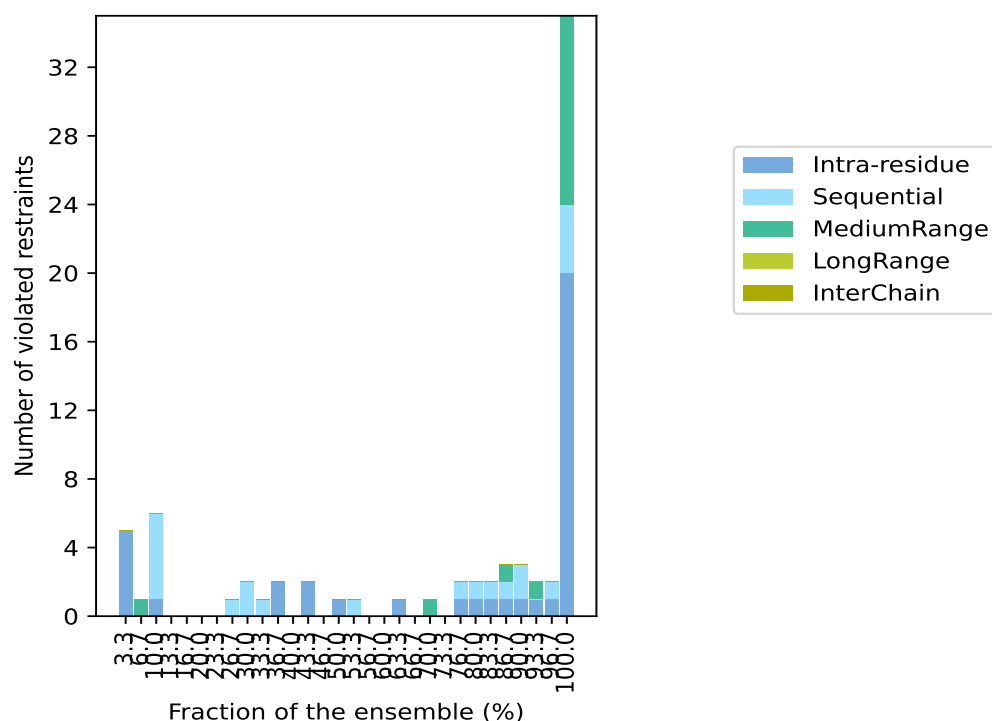
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	23.3
0	1	0	0	0	1	8	26.7
0	2	0	0	0	2	9	30.0
0	1	0	0	0	1	10	33.3
2	0	0	0	0	2	11	36.7
0	0	0	0	0	0	12	40.0
2	0	0	0	0	2	13	43.3
0	0	0	0	0	0	14	46.7
1	0	0	0	0	1	15	50.0
0	1	0	0	0	1	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
1	0	0	0	0	1	19	63.3
0	0	0	0	0	0	20	66.7
0	0	1	0	0	1	21	70.0
0	0	0	0	0	0	22	73.3
1	1	0	0	0	2	23	76.7
1	1	0	0	0	2	24	80.0
1	1	0	0	0	2	25	83.3
1	1	1	0	0	3	26	86.7
1	2	0	0	0	3	27	90.0
1	0	1	0	0	2	28	93.3
1	1	0	0	0	2	29	96.7
20	4	11	0	0	35	30	100.0

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

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

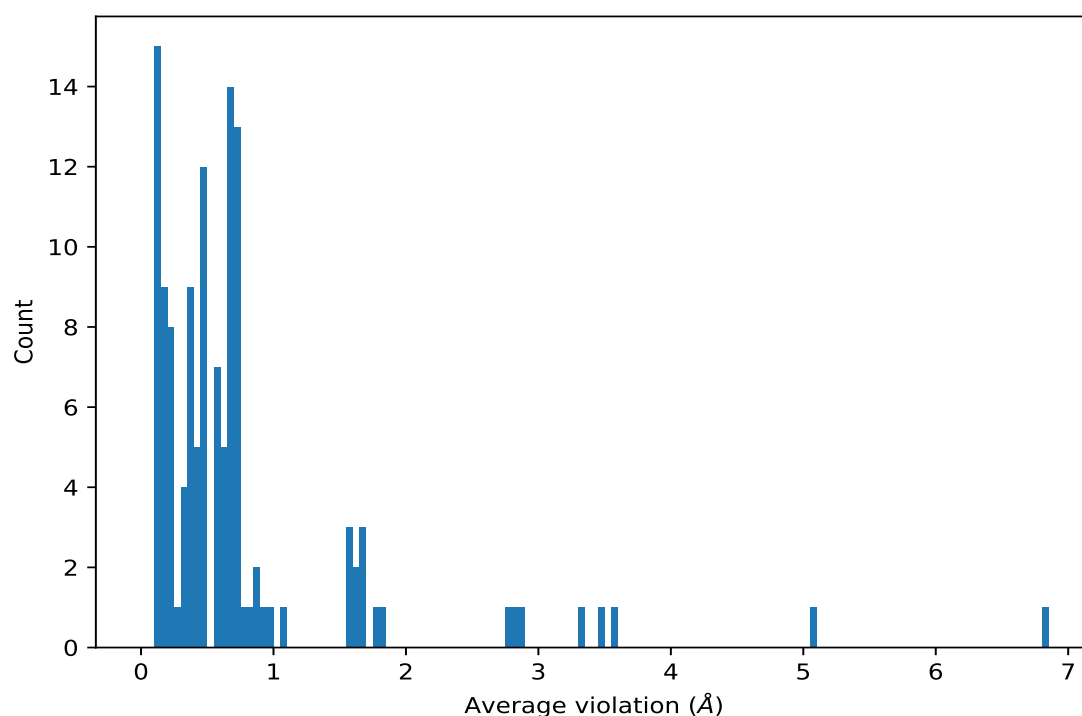
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	30	6.8	0.83	6.61
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	30	5.06	0.78	4.89
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	30	3.58	0.37	3.51
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	30	3.45	0.58	3.64
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	30	3.32	0.08	3.33
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	30	2.85	0.95	2.28
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	30	2.84	0.1	2.85
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	30	2.75	0.76	2.44
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	30	1.84	0.5	1.76
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	30	1.75	0.22	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	30	1.68	0.06	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	30	1.68	0.06	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	30	1.68	0.06	1.69
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	30	1.56	0.46	1.67
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	30	1.56	0.46	1.67
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	30	1.55	0.36	1.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	30	1.09	0.37	1.05
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	30	0.95	0.13	0.96
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	30	0.83	0.01	0.82
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	30	0.71	0.0	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	30	0.71	0.0	0.71
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	30	0.69	0.0	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	30	0.69	0.0	0.69
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	30	0.69	0.26	0.61
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	30	0.67	0.0	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	30	0.67	0.0	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	30	0.65	0.07	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	30	0.65	0.07	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	30	0.64	0.02	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	30	0.64	0.02	0.64
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	30	0.6	0.11	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	30	0.6	0.11	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	30	0.57	0.01	0.57
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	30	0.56	0.29	0.59
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	30	0.47	0.02	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	30	0.47	0.02	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	30	0.47	0.02	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	30	0.47	0.02	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	30	0.47	0.02	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	30	0.47	0.02	0.48
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	30	0.46	0.01	0.46
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	30	0.44	0.02	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	30	0.44	0.02	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	30	0.44	0.02	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	30	0.44	0.02	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	30	0.39	0.13	0.41
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	30	0.39	0.13	0.41
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	30	0.39	0.12	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	30	0.39	0.12	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	30	0.37	0.01	0.37
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	30	0.36	0.06	0.36
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	30	0.36	0.06	0.36
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	30	0.32	0.01	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	30	0.32	0.01	0.32
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	30	0.25	0.01	0.26
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	30	0.23	0.0	0.23
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	30	0.21	0.01	0.22
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	30	0.15	0.02	0.15
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	29	0.63	0.08	0.66
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	29	0.14	0.01	0.14
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	28	1.63	0.74	1.37
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	28	1.63	0.74	1.37
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	28	0.23	0.03	0.24
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	27	0.71	0.02	0.71
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	27	0.16	0.01	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	27	0.15	0.01	0.15
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	26	0.93	0.71	0.6
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	26	0.89	0.24	0.88
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	26	0.89	0.24	0.88
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	26	0.13	0.06	0.11
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	25	0.23	0.07	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	25	0.23	0.07	0.27
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	25	0.12	0.01	0.11

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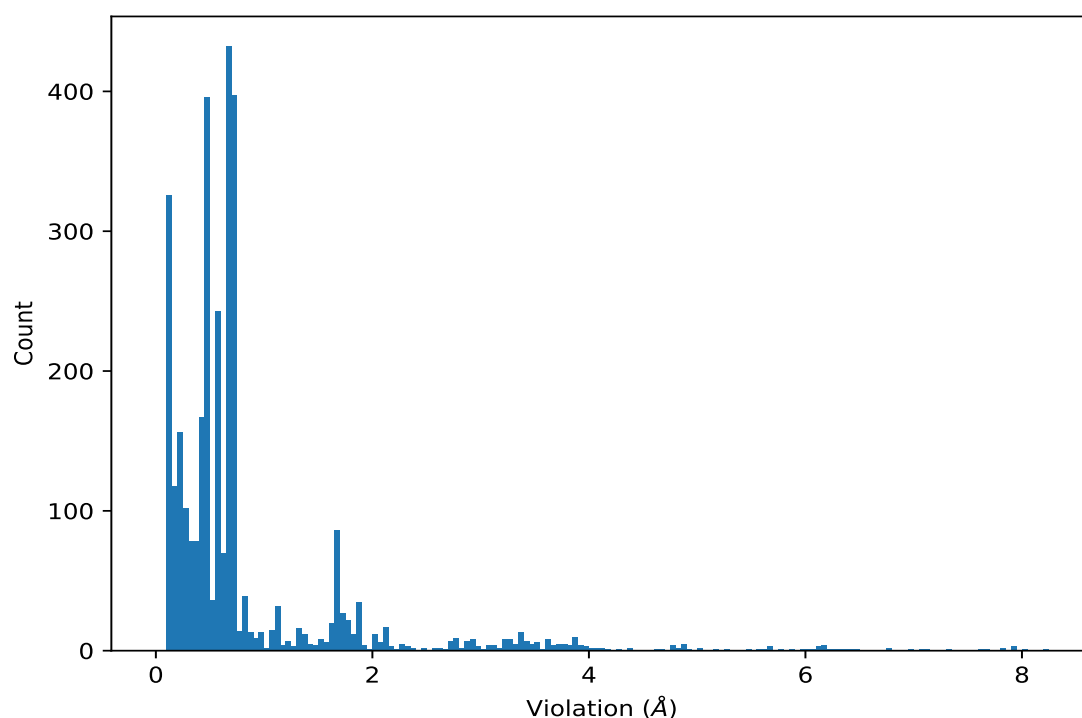
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	24	0.12	0.0	0.12
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	24	0.1	0.01	0.1
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	23	0.12	0.01	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	23	0.11	0.01	0.11
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	21	0.19	0.1	0.17
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	19	0.23	0.01	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	19	0.23	0.01	0.23
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	16	0.24	0.1	0.24
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	15	0.13	0.01	0.12
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	13	0.16	0.0	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	13	0.16	0.0	0.16
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	13	0.13	0.02	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	11	0.12	0.02	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	11	0.12	0.02	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	11	0.1	0.0	0.1
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	10	0.13	0.02	0.12
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	9	0.43	0.1	0.44
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	9	0.12	0.03	0.11
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	8	0.11	0.01	0.11
(2,91)	1:14:A:SER:H	1:15:A:SER:H	3	0.78	0.08	0.84
(2,27)	1:5:A:PHE:HD1	1:5:A:PHE:HA	3	0.35	0.04	0.36
(2,27)	1:5:A:PHE:HD2	1:5:A:PHE:HA	3	0.35	0.04	0.36
(2,79)	1:2:A:VAL:H	1:3:A:HIS:H	3	0.3	0.2	0.17
(2,92)	1:15:A:SER:H	1:16:A:SER:H	3	0.3	0.02	0.31
(2,89)	1:12:A:ASN:H	1:13:A:SER:H	3	0.19	0.01	0.18
(2,83)	1:6:A:ARG:H	1:7:A:GLY:H	3	0.16	0.06	0.14
(2,131)	1:14:A:SER:H	1:11:A:HIS:HA	2	0.16	0.01	0.16

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	9	8.24
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	11	8.04
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	4	7.94
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	28	7.94
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	3	7.92
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	5	7.84
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	21	7.82
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	8	7.66
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	24	7.61
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	6	7.31
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	27	7.11
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	13	7.08
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	23	6.96
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	14	6.8
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	18	6.75
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	20	6.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	7	6.41
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	21	6.36
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	15	6.35
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	30	6.26
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	25	6.2
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	27	6.19
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	18	6.18
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	17	6.17
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	1	6.16
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	26	6.14
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	12	6.13
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	6	6.12
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	29	6.08
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	19	6.01
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	10	5.99
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	16	5.88
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	10	5.75
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	1	5.69
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	12	5.68
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	19	5.68
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	26	5.62
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	22	5.57
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	29	5.47
(1,1)	1:3:A:HIS:O	1:7:A:GLY:H	2	5.28
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	2	5.17
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	14	5.05
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	30	5.01
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	23	4.92
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	7	4.89
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	20	4.89
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	24	4.87
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	4	4.86
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	28	4.86
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	8	4.85
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	5	4.84
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	9	4.8
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	17	4.79
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	25	4.79
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	3	4.78
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	11	4.66
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	15	4.64
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	10	4.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	24	4.37
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	27	4.25
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	22	4.18
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	16	4.14
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	21	4.11
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	18	4.09
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	6	4.08
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	29	4.02
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	26	4.02
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	26	3.99
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	11	3.97
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	12	3.95
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	19	3.94
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	13	3.94
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	9	3.93
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	1	3.91
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	4	3.9
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	28	3.9
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	15	3.89
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	27	3.87
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	6	3.86
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	19	3.86
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	28	3.86
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	3	3.85
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	5	3.85
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	29	3.85
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	7	3.84
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	8	3.82
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	21	3.82
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	5	3.81
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	10	3.8
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	24	3.79
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	9	3.78
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	2	3.75
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	13	3.75
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	6	3.71
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	14	3.7
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	20	3.7
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	23	3.7
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	16	3.7
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	27	3.67
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	16	3.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	16	3.66
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	21	3.66
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	11	3.65
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	18	3.64
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	7	3.63
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	5	3.63
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	28	3.63
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	17	3.63
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	4	3.62
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	3	3.61
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	24	3.57
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	8	3.55
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	13	3.54
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	30	3.54
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	30	3.53
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	6	3.51
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	21	3.5
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	12	3.48
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	13	3.46
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	22	3.45
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	4	3.45
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	18	3.45
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	22	3.44
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	15	3.44
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	25	3.43
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	2	3.42
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	16	3.42
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	12	3.41
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	19	3.41
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	3	3.4
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	27	3.4
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	14	3.39
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	20	3.39
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	5	3.38
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	7	3.38
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	23	3.38
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	8	3.37
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	23	3.37
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	9	3.36
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	25	3.36
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	17	3.35
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	30	3.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	10	3.34
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	14	3.33
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	10	3.31
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	13	3.31
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	25	3.31
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	24	3.3
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	17	3.3
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	4	3.27
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	11	3.26
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	18	3.26
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	1	3.25
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	8	3.25
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	28	3.25
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	6	3.24
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	15	3.24
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	21	3.24
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	27	3.24
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	1	3.23
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	12	3.21
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	19	3.21
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	26	3.21
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	1	3.18
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	2	3.17
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	29	3.15
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	26	3.14
(2,140)	1:11:A:HIS:HA	1:8:A:ILE:HB	29	3.11
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	22	3.1
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	11	3.07
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	20	3.07
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	3	3.06
(1,2)	1:13:A:SER:O	1:17:A:LEU:H	9	3.06
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	2	3.05
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	6	2.97
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	26	2.97
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	10	2.96
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	12	2.94
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	16	2.94
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	19	2.94
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	26	2.93
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	17	2.92
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	18	2.92
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	30	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	25	2.91
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	1	2.9
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	21	2.9
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	27	2.89
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	2	2.89
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	24	2.88
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	10	2.87
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	29	2.87
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	22	2.83
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	11	2.82
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	14	2.79
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	5	2.77
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	7	2.77
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	15	2.76
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	20	2.76
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	4	2.75
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	9	2.75
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	24	2.75
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	28	2.75
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	8	2.74
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	23	2.74
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	21	2.73
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	21	2.73
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	3	2.72
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	18	2.7
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	18	2.7
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	22	2.66
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	14	2.62
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	18	2.6
(2,128)	1:9:A:ASN:H	1:6:A:ARG:HA	13	2.58
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	23	2.57
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	2	2.46
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	2	2.46
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	30	2.39
(2,135)	1:8:A:ILE:H	1:4:A:THR:HA	16	2.37
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	16	2.31
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	22	2.31
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	30	2.31
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	20	2.29
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	17	2.28
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	7	2.28
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	25	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	15	2.26
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	14	2.21
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	26	2.16
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	26	2.16
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	13	2.16
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	6	2.14
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	27	2.14
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	28	2.14
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	25	2.13
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	1	2.12
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	1	2.12
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	19	2.12
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	19	2.12
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	16	2.12
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	5	2.12
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	29	2.12
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	17	2.11
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	12	2.1
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	12	2.1
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	15	2.1
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	1	2.1
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	26	2.1
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	13	2.09
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	23	2.09
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	12	2.09
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	19	2.08
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	7	2.07
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	16	2.06
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	10	2.05
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	10	2.05
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	29	2.05
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	29	2.05
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	20	2.05
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	29	2.05
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	7	2.04
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	4	2.03
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	28	2.03
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	15	2.02
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	5	2.01
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	8	2.01
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	24	1.96
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	27	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	27	1.95
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	16	1.93
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	27	1.92
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	6	1.9
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	6	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	6	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	7	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	8	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	9	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	13	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	14	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	17	1.9
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	25	1.9
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	30	1.89
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	3	1.89
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	12	1.89
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	19	1.89
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	23	1.89
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	26	1.89
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	19	1.88
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	6	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	6	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	17	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	17	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	27	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	27	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	28	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	28	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	30	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	30	1.87
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	5	1.86
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	5	1.86
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	29	1.86
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	29	1.86
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	11	1.86
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	3	1.85
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	14	1.85
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	22	1.85
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	23	1.84
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	17	1.83
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	18	1.83
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	11	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	15	1.82
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	13	1.81
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	13	1.81
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	15	1.81
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	15	1.81
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	10	1.81
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	7	1.81
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	20	1.81
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	19	1.79
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	19	1.79
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	6	1.79
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	18	1.79
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	21	1.79
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	21	1.78
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	21	1.78
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	21	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	1	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	17	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	25	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	26	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	29	1.78
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	12	1.77
(2,136)	1:9:A:ASN:H	1:5:A:PHE:HA	9	1.76
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	9	1.76
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	12	1.75
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	12	1.75
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	12	1.75
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	30	1.75
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	10	1.75
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	19	1.75
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	11	1.73
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	11	1.73
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	11	1.73
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	9	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	9	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	9	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	15	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	15	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	15	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	30	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	30	1.72
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	30	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	10	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	10	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	10	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	16	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	16	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	16	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	17	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	17	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	17	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	21	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	21	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	21	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	25	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	25	1.71
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	25	1.71
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	1	1.7
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	1	1.7
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	7	1.7
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	7	1.7
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	4	1.7
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	18	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	1	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	4	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	5	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	11	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	15	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	16	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	20	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	21	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	22	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	27	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	28	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	29	1.7
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	30	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	6	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	6	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	6	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	27	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	27	1.7
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	27	1.7
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	2	1.69
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	8	1.69
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	23	1.69
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	2	1.69
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	10	1.69
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	24	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	2	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	2	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	2	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	3	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	3	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	3	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	8	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	8	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	8	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	12	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	12	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	12	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	13	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	13	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	13	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	18	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	18	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	18	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	19	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	19	1.69
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	19	1.69
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	25	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	1	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	1	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	1	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	24	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	24	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	24	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	28	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	28	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	28	1.68
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	4	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	4	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	4	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	5	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	5	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	5	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	7	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	7	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	7	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	20	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	20	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	20	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	23	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	23	1.67
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	23	1.67
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	8	1.66
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	1	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	14	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	14	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	14	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	22	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	22	1.66
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	22	1.66
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	4	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	4	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	16	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	16	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	18	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	18	1.65
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	25	1.63
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	25	1.63
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	12	1.63
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	8	1.62
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	8	1.62
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	19	1.62
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	2	1.62
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	13	1.62
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	23	1.61
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	23	1.61
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	26	1.61
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	20	1.6
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	20	1.6
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	14	1.6
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	3	1.55
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	3	1.55
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	9	1.55
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	9	1.55
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	11	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	11	1.55
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	10	1.54
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	6	1.53
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	27	1.53
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	29	1.53
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	29	1.53
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	29	1.53
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	22	1.52
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	22	1.52
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	14	1.49
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	14	1.49
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	29	1.48
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	2	1.47
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	10	1.44
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	24	1.44
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD11	26	1.42
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD12	26	1.42
(2,42)	1:8:A:ILE:H	1:8:A:ILE:HD13	26	1.42
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	14	1.4
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	14	1.4
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	30	1.4
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	26	1.38
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	4	1.37
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	4	1.37
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	28	1.37
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	28	1.37
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	5	1.35
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	5	1.35
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	23	1.35
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	23	1.35
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	24	1.34
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	8	1.33
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	8	1.33
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	20	1.33
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	20	1.33
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	24	1.33
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	24	1.33
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	21	1.33
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	8	1.32
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	7	1.31
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	7	1.31
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	27	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	24	1.31
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	4	1.3
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	5	1.3
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	28	1.3
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	3	1.29
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	3	1.29
(2,125)	1:6:A:ARG:H	1:3:A:HIS:HA	2	1.28
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	5	1.23
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	3	1.23
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	3	1.22
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	4	1.21
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	21	1.21
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	28	1.21
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	1	1.21
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	2	1.2
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	7	1.19
(2,23)	1:4:A:THR:H	1:4:A:THR:HB	23	1.19
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	22	1.16
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	17	1.15
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	17	1.15
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	9	1.15
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	6	1.14
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	3	1.14
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	11	1.13
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	20	1.13
(2,132)	1:17:A:LEU:H	1:14:A:SER:HA	22	1.13
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	13	1.12
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	6	1.12
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	6	1.12
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	26	1.12
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	26	1.12
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	2	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	2	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	4	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	4	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	13	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	13	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	17	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	17	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	20	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	20	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	22	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	22	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	25	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	25	1.11
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	28	1.11
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	28	1.11
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	20	1.1
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	9	1.1
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	9	1.1
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	25	1.09
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	25	1.09
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	17	1.08
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	13	1.07
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	16	1.07
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	11	1.07
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	5	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	6	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	7	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	15	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	19	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	27	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	28	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	29	1.06
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	30	1.06
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	9	1.02
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	15	1.0
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	26	0.98
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	13	0.97
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	8	0.97
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	12	0.97
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	21	0.97
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	16	0.96
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	16	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	4	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	8	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	14	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	18	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	23	0.96
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	25	0.96
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	12	0.95
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	25	0.95
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	17	0.94
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	11	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	11	0.93
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	10	0.92
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	22	0.92
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	1	0.91
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	26	0.9
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	18	0.89
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	24	0.89
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	10	0.88
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	7	0.88
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	7	0.88
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	14	0.87
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	14	0.87
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	24	0.87
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	24	0.87
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	30	0.86
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	30	0.86
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	29	0.86
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	26	0.86
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	3	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	9	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	10	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	11	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	16	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	20	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	22	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	24	0.84
(2,91)	1:14:A:SER:H	1:15:A:SER:H	10	0.84
(2,91)	1:14:A:SER:H	1:15:A:SER:H	24	0.84
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	12	0.83
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	14	0.83
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	17	0.83
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	19	0.83
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	29	0.83
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	30	0.83
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	22	0.83
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	22	0.83
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	27	0.82
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	27	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	1	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	2	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	4	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	5	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	6	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	7	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	8	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	13	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	15	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	18	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	21	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	23	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	25	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	27	0.82
(2,104)	1:12:A:ASN:H	1:11:A:HIS:HA	28	0.82
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	1	0.8
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	1	0.8
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	18	0.8
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	18	0.8
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	24	0.78
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	24	0.78
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	22	0.77
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	12	0.77
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	12	0.77
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	19	0.77
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	19	0.77
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	30	0.75
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	14	0.75
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	9	0.75
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	20	0.75
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	22	0.75
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	11	0.75
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	11	0.75
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	3	0.74
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	9	0.74
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	11	0.74
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	20	0.74
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	22	0.74
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	3	0.74
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	11	0.74
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	3	0.74
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	3	0.74
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	13	0.74
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	13	0.74
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	24	0.73
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	30	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	30	0.73
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	23	0.73
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	21	0.73
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	21	0.73
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	27	0.73
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	27	0.73
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	15	0.73
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	15	0.73
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	2	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	4	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	8	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	16	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	17	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	25	0.72
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	1	0.72
(2,93)	1:16:A:SER:H	1:17:A:LEU:H	2	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	28	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	28	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	30	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	30	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	30	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	30	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	30	0.72
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	30	0.72
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	30	0.72
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	1	0.71
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	18	0.71
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	30	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	1	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	1	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	2	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	2	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	3	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	3	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	4	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	4	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	4	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	4	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	4	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	4	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	5	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	5	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	6	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	6	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	7	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	7	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	7	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	7	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	7	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	7	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	7	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	8	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	8	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	9	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	9	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	10	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	10	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	11	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	11	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	11	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	11	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	11	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	11	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	11	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	12	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	12	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	13	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	13	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	14	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	14	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	14	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	14	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	14	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	14	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	14	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	15	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	15	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	16	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	16	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	17	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	17	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	18	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	18	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	18	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	18	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	18	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	18	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	18	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	19	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	19	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	20	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	20	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	21	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	21	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	21	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	21	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	21	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	21	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	21	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	22	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	22	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	23	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	23	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	24	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	24	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	25	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	25	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	25	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	25	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	25	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	25	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	25	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	26	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	26	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	27	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	27	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD11	29	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD12	29	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD13	29	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD11	29	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD12	29	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD13	29	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD21	29	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD22	29	0.71
(2,76)	1:17:A:LEU:HB2	1:17:A:LEU:HD23	29	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD21	29	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD22	29	0.71
(2,76)	1:17:A:LEU:HB3	1:17:A:LEU:HD23	29	0.71
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	8	0.71
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	8	0.71
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	5	0.71
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	5	0.71
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	12	0.7
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	15	0.7
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	19	0.7
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	21	0.7
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	3	0.7
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	9	0.7
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	14	0.69
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	20	0.69
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	20	0.69
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	13	0.69
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	2	0.69
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	11	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	1	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	1	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	1	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	1	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	1	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	1	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	1	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	1	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	1	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	2	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	2	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	2	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	2	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	2	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	2	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	2	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	2	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	2	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	3	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	3	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	3	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	3	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	3	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	3	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	3	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	3	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	4	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	4	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	4	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	4	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	4	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	4	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	4	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	4	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	4	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	5	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	5	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	5	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	5	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	5	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	5	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	5	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	5	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	5	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	6	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	6	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	6	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	6	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	6	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	6	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	6	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	6	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	6	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	7	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	7	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	7	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	7	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	7	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	7	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	7	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	7	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	7	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	8	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	8	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	8	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	8	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	8	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	8	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	8	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	8	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	9	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	9	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	9	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	9	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	9	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	9	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	9	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	9	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	9	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	10	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	10	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	10	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	10	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	10	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	10	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	10	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	10	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	10	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	11	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	11	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	11	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	11	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	11	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	11	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	11	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	11	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	11	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	12	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	12	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	12	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	12	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	12	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	12	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	12	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	12	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	12	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	13	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	13	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	13	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	13	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	13	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	13	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	13	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	13	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	13	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	14	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	14	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	14	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	14	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	14	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	14	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	14	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	14	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	14	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	15	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	15	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	15	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	15	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	15	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	15	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	15	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	15	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	15	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	16	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	16	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	16	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	16	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	16	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	16	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	16	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	16	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	16	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	17	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	17	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	17	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	17	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	17	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	17	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	17	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	17	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	18	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	18	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	18	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	18	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	18	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	18	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	18	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	18	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	18	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	19	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	19	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	19	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	19	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	19	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	19	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	19	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	19	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	19	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	20	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	20	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	20	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	20	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	20	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	20	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	20	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	20	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	20	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	21	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	21	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	21	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	21	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	21	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	21	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	21	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	21	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	21	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	22	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	22	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	22	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	22	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	22	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	22	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	22	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	22	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	22	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	23	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	23	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	23	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	23	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	23	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	23	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	23	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	23	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	23	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	24	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	24	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	24	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	24	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	24	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	24	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	24	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	24	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	24	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	25	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	25	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	25	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	25	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	25	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	25	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	25	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	25	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	25	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	26	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	26	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	26	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	26	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	26	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	26	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	26	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	26	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	26	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	27	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	27	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	27	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	27	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	27	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	27	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	27	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	27	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	27	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	28	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	28	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	28	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	28	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	28	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	28	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	28	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	28	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	28	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	29	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	29	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	29	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	29	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	29	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	29	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	29	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	29	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	29	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD11	30	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD12	30	0.69
(2,78)	1:17:A:LEU:HD21	1:17:A:LEU:HD13	30	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD11	30	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD12	30	0.69
(2,78)	1:17:A:LEU:HD22	1:17:A:LEU:HD13	30	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD11	30	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD12	30	0.69
(2,78)	1:17:A:LEU:HD23	1:17:A:LEU:HD13	30	0.69
(2,52)	1:9:A:ASN:HD22	1:9:A:ASN:HA	18	0.69
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	11	0.69
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	11	0.69
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	10	0.69
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	10	0.69
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	20	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	20	0.69
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	19	0.68
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	5	0.68
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	6	0.68
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	27	0.68
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	28	0.68
(2,108)	1:16:A:SER:H	1:15:A:SER:HA	29	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	4	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	4	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	6	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	6	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	9	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	9	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	28	0.68
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	28	0.68
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	15	0.67
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	21	0.67
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	4	0.67
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	5	0.67
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	24	0.67
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	28	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	1	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	1	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	2	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	2	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	3	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	3	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	4	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	4	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	5	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	5	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	6	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	6	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	8	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	8	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	9	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	9	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	10	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	10	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	11	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	11	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	12	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	12	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	13	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	13	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	14	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	14	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	15	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	15	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	16	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	16	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	17	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	17	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	18	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	18	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	19	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	19	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	20	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	20	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	21	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	21	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	22	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	22	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	23	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	23	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	24	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	24	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	25	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	25	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	26	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	26	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	27	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	27	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	28	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	28	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	29	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	29	0.67
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	30	0.67
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	30	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	7	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	7	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	14	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	14	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	17	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	17	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	25	0.67
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	25	0.67
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	6	0.66
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	27	0.66
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	28	0.66
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	7	0.66
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	7	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	1	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	8	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	10	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	12	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	17	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	19	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	21	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	25	0.66
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	26	0.66
(2,91)	1:14:A:SER:H	1:15:A:SER:H	26	0.66
(2,75)	1:17:A:LEU:HB2	1:17:A:LEU:HG	7	0.66
(2,75)	1:17:A:LEU:HB3	1:17:A:LEU:HG	7	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	1	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	1	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	6	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	6	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	13	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	13	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	26	0.66
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	26	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	2	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	2	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	23	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	23	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	26	0.66
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	26	0.66
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	27	0.65
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	23	0.65
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	23	0.65
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	29	0.65
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	24	0.65
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	24	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	9	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	10	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	10	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	15	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	15	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	17	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	17	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	21	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	21	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	24	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	24	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	25	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	25	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	27	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	27	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	30	0.65
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	30	0.65
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	24	0.65
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	24	0.65
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	1	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	2	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	12	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	15	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	17	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	25	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	26	0.64
(2,126)	1:7:A:GLY:H	1:4:A:THR:HA	16	0.64
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	15	0.64
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	10	0.64
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	10	0.64
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	26	0.64
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	26	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	4	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	4	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	5	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	5	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	7	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	7	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	8	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	8	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	20	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	20	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	23	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	23	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	28	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	28	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	29	0.64
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	29	0.64
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	16	0.64
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	16	0.64
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	19	0.63
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	20	0.63
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	8	0.63
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	14	0.63
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	14	0.63
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	18	0.63
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	18	0.63
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	1	0.63
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	1	0.63
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	1	0.62
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	4	0.62
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	18	0.62
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	16	0.62
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	29	0.62
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	7	0.62
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	18	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	2	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	2	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	3	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	3	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	12	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	12	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	16	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	16	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	19	0.62
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	19	0.62
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	2	0.61
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	5	0.61
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	7	0.61
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	12	0.61
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	19	0.61
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	22	0.61
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	22	0.61
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	12	0.61
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	12	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	18	0.61
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	18	0.61
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	19	0.61
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	19	0.61
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	8	0.6
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	25	0.6
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	29	0.6
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	21	0.6
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	21	0.6
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	30	0.6
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	23	0.59
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	23	0.59
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB2	22	0.59
(2,50)	1:9:A:ASN:H	1:9:A:ASN:HB3	22	0.59
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	8	0.59
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	8	0.59
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	8	0.59
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	8	0.59
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	8	0.59
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	8	0.59
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	8	0.59
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	8	0.59
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	1	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	1	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	4	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	4	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	5	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	5	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	11	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	11	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	26	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	26	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	28	0.58
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	28	0.58
(2,79)	1:2:A:VAL:H	1:3:A:HIS:H	8	0.58
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	3	0.58
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	3	0.58
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	27	0.58
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	27	0.58
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	22	0.58
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	22	0.58
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	22	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	22	0.58
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	22	0.58
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	22	0.58
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	3	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	3	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	9	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	9	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	10	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	10	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	12	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	12	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	15	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	15	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	17	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	17	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	19	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	19	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	25	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	25	0.57
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	29	0.57
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	29	0.57
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	14	0.57
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	24	0.57
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	24	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	3	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	4	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	5	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	5	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	5	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	5	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	5	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	6	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	7	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	9	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	10	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	11	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	12	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	13	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	13	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	13	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	13	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	13	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	14	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	15	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	17	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	18	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	20	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	21	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	23	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	23	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	23	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	23	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	23	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	23	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	24	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	25	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	26	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	27	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	28	0.57
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	29	0.57
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	29	0.57
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	29	0.57
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	29	0.57
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	29	0.57
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	29	0.57
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	9	0.56
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	9	0.56
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	16	0.56
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	13	0.56
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	27	0.56
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	10	0.56
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	1	0.56
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	2	0.56
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	16	0.56
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	19	0.56
(2,20)	1:2:A:VAL:HG11	1:2:A:VAL:HA	30	0.56
(2,20)	1:2:A:VAL:HG12	1:2:A:VAL:HA	30	0.56
(2,20)	1:2:A:VAL:HG13	1:2:A:VAL:HA	30	0.56
(2,20)	1:2:A:VAL:HG21	1:2:A:VAL:HA	30	0.56
(2,20)	1:2:A:VAL:HG22	1:2:A:VAL:HA	30	0.56
(2,20)	1:2:A:VAL:HG23	1:2:A:VAL:HA	30	0.56
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	6	0.55
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	6	0.55
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	6	0.55
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	13	0.55
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	13	0.55
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	6	0.55
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	11	0.54
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	14	0.54
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	20	0.54
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	16	0.54
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	21	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	21	0.54
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	30	0.54
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	30	0.54
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	3	0.53
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	9	0.53
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	18	0.53
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	2	0.53
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	2	0.53
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	18	0.53
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	18	0.53
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	29	0.53
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	29	0.53
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	17	0.51
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	30	0.51
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	7	0.51
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	10	0.51
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	21	0.51
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	21	0.51
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	14	0.5
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	14	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	10	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	10	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	10	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	10	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	10	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	10	0.5
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	12	0.5
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	12	0.5
(2,56)	1:12:A:ASN:HD22	1:12:A:ASN:HA	11	0.5
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB2	16	0.5
(2,29)	1:6:A:ARG:H	1:6:A:ARG:HB3	16	0.5
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	4	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	8	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	8	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	8	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	8	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	8	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	12	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	14	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	18	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	23	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	24	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	25	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	25	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	25	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	25	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	25	0.49
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	25	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	4	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	4	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	8	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	8	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	18	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	23	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	23	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	25	0.49
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	25	0.49
(2,138)	1:15:A:SER:H	1:11:A:HIS:HA	22	0.48
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	11	0.48
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	7	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	13	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	15	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	16	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	17	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	21	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	21	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	21	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	21	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	21	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	21	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	26	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	27	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	27	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	27	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	27	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	27	0.48
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	27	0.48
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	10	0.48
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	10	0.48
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	10	0.48
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	10	0.48
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	29	0.48
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	29	0.48
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	29	0.48
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	29	0.48
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	29	0.48
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	29	0.48
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	3	0.47
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	10	0.47
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	12	0.47
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	12	0.47
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	12	0.47
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	12	0.47
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	12	0.47
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	24	0.47
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	24	0.47
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	24	0.47
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	24	0.47
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	24	0.47
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	24	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	5	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	6	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	19	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	28	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	29	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	30	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	30	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	30	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	30	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	30	0.47
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	30	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	14	0.47
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	14	0.47
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	30	0.47
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	30	0.47
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	30	0.47
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	30	0.47
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	9	0.46
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	7	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	1	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	2	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	4	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	8	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	9	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	11	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	11	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	11	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	11	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	11	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	13	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	14	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	15	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	16	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	17	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	18	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	20	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	20	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	20	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	20	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	20	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	20	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	21	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	22	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	23	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	25	0.46
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	26	0.46
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	26	0.46
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	26	0.46
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	26	0.46
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	26	0.46
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	26	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	4	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	4	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	18	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	18	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	25	0.46
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	25	0.46
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	5	0.46
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	5	0.46
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	20	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	5	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	5	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	5	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	5	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	5	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	6	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	7	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	19	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	27	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	28	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	29	0.45
(2,74)	1:17:A:LEU:HD11	1:17:A:LEU:HA	30	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:17:A:LEU:HD12	1:17:A:LEU:HA	30	0.45
(2,74)	1:17:A:LEU:HD13	1:17:A:LEU:HA	30	0.45
(2,74)	1:17:A:LEU:HD21	1:17:A:LEU:HA	30	0.45
(2,74)	1:17:A:LEU:HD22	1:17:A:LEU:HA	30	0.45
(2,74)	1:17:A:LEU:HD23	1:17:A:LEU:HA	30	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	3	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	22	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	22	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	22	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	22	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	22	0.45
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	22	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	2	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	2	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	7	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	7	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	12	0.45
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	12	0.45
(2,55)	1:11:A:HIS:HB2	1:11:A:HIS:HD2	26	0.45
(2,55)	1:11:A:HIS:HB3	1:11:A:HIS:HD2	26	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	9	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	9	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	9	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	9	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	16	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	16	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	16	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	16	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	22	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	22	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	22	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	22	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	25	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	25	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	25	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	25	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	27	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	27	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	27	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	27	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	28	0.45
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	28	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	28	0.45
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	28	0.45
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	23	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	9	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	11	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	20	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	20	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	20	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	20	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	20	0.44
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	20	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	3	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	3	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	9	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	9	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	26	0.44
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	26	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	1	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	1	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	19	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	19	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	21	0.44
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	21	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	2	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	2	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	2	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	4	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	4	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	4	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	4	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	6	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	6	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	6	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	6	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	13	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	13	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	13	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	13	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	17	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	17	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	17	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	17	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	20	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	20	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	20	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	20	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	21	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	21	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	21	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	21	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	23	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	23	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	23	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	23	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	26	0.44
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	26	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	26	0.44
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	26	0.44
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	15	0.44
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	15	0.44
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	9	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	1	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD11	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD12	2	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD13	2	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD21	2	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD22	2	0.43
(2,71)	1:17:A:LEU:H	1:17:A:LEU:HD23	2	0.43
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	22	0.43
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	22	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	8	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	8	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	8	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	8	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	12	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	12	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	12	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	12	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	19	0.43
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	19	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	19	0.43
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	19	0.43
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	2	0.42
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	14	0.42
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	15	0.42
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	15	0.42
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	30	0.42
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	30	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	1	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	1	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	1	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	1	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	3	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	3	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	3	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	3	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	15	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	15	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	15	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	15	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	18	0.42
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	18	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	18	0.42
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	18	0.42
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	8	0.42
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	23	0.42
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	23	0.42
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	29	0.42
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	29	0.42
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	30	0.41
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	17	0.41
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	17	0.41
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	22	0.41
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	22	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	5	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	5	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	5	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	5	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	7	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	7	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	7	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	7	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	14	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	14	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	14	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	14	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	24	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	24	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	24	0.41
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	24	0.41
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	1	0.41
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	1	0.41
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	3	0.41
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	3	0.41
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	14	0.41
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	14	0.41
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	19	0.41
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	19	0.41
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB2	11	0.4
(2,35)	1:6:A:ARG:HD2	1:6:A:ARG:HB3	11	0.4
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB2	11	0.4
(2,35)	1:6:A:ARG:HD3	1:6:A:ARG:HB3	11	0.4
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	7	0.4
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	7	0.4
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	11	0.4
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	12	0.4
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	12	0.4
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	18	0.4
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	18	0.4
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	24	0.4
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	24	0.4
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	14	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	5	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	5	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	23	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	23	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	29	0.39
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	29	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	4	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	5	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	8	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	14	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	20	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	23	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	24	0.39
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	28	0.39
(2,27)	1:5:A:PHE:HD1	1:5:A:PHE:HA	11	0.39
(2,27)	1:5:A:PHE:HD2	1:5:A:PHE:HA	11	0.39
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	30	0.38
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	24	0.38
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	8	0.38
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	8	0.38
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	13	0.38
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	13	0.38
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	3	0.38
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	7	0.38
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	13	0.38
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	15	0.38
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	22	0.38
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	5	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	5	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	6	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	6	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	27	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	27	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	28	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	28	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	29	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	29	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	30	0.37
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	30	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	6	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	6	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	27	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	27	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	28	0.37
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	28	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	1	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	6	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	9	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	10	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	11	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	17	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	18	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	25	0.37
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	30	0.37
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	27	0.37
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	27	0.37
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	23	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	1	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	1	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	2	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	2	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	11	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	11	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	20	0.36
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	20	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	2	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	12	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	19	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	21	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	26	0.36
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	27	0.36
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	21	0.36
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	21	0.36
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	30	0.36
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	30	0.36
(2,27)	1:5:A:PHE:HD1	1:5:A:PHE:HA	9	0.36
(2,27)	1:5:A:PHE:HD2	1:5:A:PHE:HA	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	11	0.35
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	21	0.35
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	27	0.35
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	16	0.35
(2,40)	1:8:A:ILE:H	1:8:A:ILE:HB	29	0.35
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	10	0.35
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	10	0.35
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	16	0.35
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	16	0.35
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	29	0.34
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	29	0.34
(2,134)	1:6:A:ARG:H	1:2:A:VAL:HA	23	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	3	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	3	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	4	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	4	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	5	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	5	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	7	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	7	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	8	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	8	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	13	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	13	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	14	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	14	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	16	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	16	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	20	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	20	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	22	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	22	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	23	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	23	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	24	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	24	0.33
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	28	0.33
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	28	0.33
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	26	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	1	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	1	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	2	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	6	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	6	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	10	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	10	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	12	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	12	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	17	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	17	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	18	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	18	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	19	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	19	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	21	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	21	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	25	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	25	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	26	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	26	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	27	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	27	0.32
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	30	0.32
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	30	0.32
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	2	0.32
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	2	0.32
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	7	0.31
(2,92)	1:15:A:SER:H	1:16:A:SER:H	10	0.31
(2,92)	1:15:A:SER:H	1:16:A:SER:H	24	0.31
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	9	0.31
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	9	0.31
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	11	0.31
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	11	0.31
(2,44)	1:8:A:ILE:HG12	1:8:A:ILE:HA	15	0.31
(2,44)	1:8:A:ILE:HG13	1:8:A:ILE:HA	15	0.31
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	30	0.31
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	30	0.31
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	26	0.3
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	26	0.3
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	24	0.3
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	10	0.3
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	24	0.3
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	26	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	26	0.3
(2,27)	1:5:A:PHE:HD1	1:5:A:PHE:HA	16	0.3
(2,27)	1:5:A:PHE:HD2	1:5:A:PHE:HA	16	0.3
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	13	0.29
(2,116)	1:1:A:ASN:HB2	1:2:A:VAL:H	8	0.29
(2,116)	1:1:A:ASN:HB3	1:2:A:VAL:H	8	0.29
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	27	0.29
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	4	0.29
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	4	0.29
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	17	0.29
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	17	0.29
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	20	0.29
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	20	0.29
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	28	0.29
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	28	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	2	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	17	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	17	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	25	0.29
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	25	0.29
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	11	0.28
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	11	0.28
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	10	0.28
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	17	0.28
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	23	0.28
(2,98)	1:6:A:ARG:H	1:5:A:PHE:HA	22	0.28
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	6	0.28
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	6	0.28
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	9	0.28
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	9	0.28
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	13	0.28
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	13	0.28
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	25	0.28
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	25	0.28
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	26	0.28
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	26	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	4	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	6	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	6	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	9	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	23	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	23	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	28	0.28
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	28	0.28
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB2	15	0.27
(2,139)	1:8:A:ILE:HA	1:5:A:PHE:HB3	15	0.27
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	10	0.27
(2,92)	1:15:A:SER:H	1:16:A:SER:H	26	0.27
(2,34)	1:6:A:ARG:HG2	1:6:A:ARG:HA	22	0.27
(2,34)	1:6:A:ARG:HG3	1:6:A:ARG:HA	22	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	10	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	10	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	16	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	16	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	20	0.27
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	20	0.27
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	25	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	2	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	4	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	7	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	8	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	9	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	10	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	14	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	18	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	20	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	21	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	22	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	23	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	24	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	25	0.26
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	26	0.26
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	7	0.26
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	10	0.26
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	20	0.26
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	27	0.26
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	3	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	1	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	5	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	6	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	19	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	28	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	29	0.25
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	30	0.25
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	17	0.25
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	17	0.25
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	13	0.25
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	13	0.25
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	1	0.25
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	6	0.25
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	13	0.25
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	24	0.25
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	5	0.24
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	7	0.24
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	20	0.24
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	4	0.24
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	5	0.24
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	28	0.24
(2,83)	1:6:A:ARG:H	1:7:A:GLY:H	22	0.24
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	15	0.24
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	15	0.24
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	22	0.24
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	22	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	2	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	3	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	5	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	12	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	15	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	17	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	19	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	21	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	22	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	25	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	26	0.24
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	28	0.24
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	4	0.23
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	20	0.23
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	28	0.23
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	21	0.23
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	20	0.23
(2,94)	1:2:A:VAL:H	1:1:A:ASN:HA	16	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	12	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	13	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	15	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	16	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	17	0.23
(2,73)	1:17:A:LEU:HG	1:17:A:LEU:HA	27	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	1	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	2	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	3	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	4	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	5	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	6	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	7	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	8	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	9	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	10	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	11	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	12	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	13	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	14	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	15	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	16	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	17	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	18	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	19	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	20	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	21	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	22	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	23	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	24	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	25	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	26	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	27	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	28	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	29	0.23
(2,43)	1:8:A:ILE:HB	1:8:A:ILE:HA	30	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	1	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	1	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	3	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	3	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	4	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	5	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	5	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	6	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	6	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	13	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	13	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	14	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	14	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	15	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	15	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	16	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	16	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	19	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	19	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	20	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	20	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	21	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	21	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	24	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	24	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	26	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	26	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	27	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	27	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	28	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	28	0.23
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	29	0.23
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	29	0.23
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	4	0.23
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	18	0.23
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	29	0.23
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	8	0.22
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	16	0.22
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	21	0.22
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	21	0.22
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	29	0.22
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	29	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	2	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	6	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	7	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	10	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	14	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	16	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	17	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	18	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	19	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	20	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	23	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	24	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	27	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	28	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	29	0.22
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	30	0.22
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	30	0.22
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	18	0.21
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	24	0.21
(2,22)	1:3:A:HIS:HB2	1:3:A:HIS:HD2	2	0.21
(2,22)	1:3:A:HIS:HB3	1:3:A:HIS:HD2	2	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	1	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	3	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	4	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	5	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	9	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	11	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	12	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	15	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	21	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	22	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	25	0.21
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	26	0.21
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	10	0.2
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	10	0.2
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB2	24	0.2
(2,141)	1:15:A:SER:HA	1:12:A:ASN:HB3	24	0.2
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	21	0.2
(2,89)	1:12:A:ASN:H	1:13:A:SER:H	26	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	3	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	3	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	9	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	9	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	14	0.2
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	14	0.2
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	4	0.19
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	28	0.19
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	4	0.19
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	5	0.19
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	28	0.19
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	30	0.19
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	16	0.19
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	16	0.19
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	9	0.19
(2,133)	1:5:A:PHE:H	1:1:A:ASN:HA	3	0.18
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	8	0.18
(2,89)	1:12:A:ASN:H	1:13:A:SER:H	10	0.18
(2,89)	1:12:A:ASN:H	1:13:A:SER:H	24	0.18
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	22	0.18
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	22	0.18
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	27	0.18
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	27	0.18
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	11	0.18
(2,131)	1:14:A:SER:H	1:11:A:HIS:HA	24	0.17
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	5	0.17
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	3	0.17
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	14	0.17
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	22	0.17
(2,82)	1:5:A:PHE:H	1:6:A:ARG:H	16	0.17
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	22	0.17
(2,79)	1:2:A:VAL:H	1:3:A:HIS:H	11	0.17
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	19	0.17
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	19	0.17
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	7	0.17
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	7	0.17
(2,32)	1:6:A:ARG:HD2	1:6:A:ARG:HA	30	0.17
(2,32)	1:6:A:ARG:HD3	1:6:A:ARG:HA	30	0.17
(2,19)	1:2:A:VAL:HB	1:2:A:VAL:HA	8	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	1	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	2	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	3	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	9	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	11	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	20	0.17
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	22	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	1	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	6	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	13	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	15	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	16	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	17	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	19	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	21	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	27	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	28	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	29	0.17
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	30	0.17
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	30	0.17
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	23	0.17
(2,131)	1:14:A:SER:H	1:11:A:HIS:HA	10	0.16
(2,127)	1:8:A:ILE:H	1:5:A:PHE:HA	24	0.16
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	23	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	1	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	2	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	4	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	12	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	18	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	21	0.16
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	25	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	7	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	7	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	13	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	13	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB3	15	0.16
(2,68)	1:16:A:SER:H	1:16:A:SER:HB2	15	0.16
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	13	0.16
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	13	0.16
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	11	0.16
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	11	0.16
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	20	0.16
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	20	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	3	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	3	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	6	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	6	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	8	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	8	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	9	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	12	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	12	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	13	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	13	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	14	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	14	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	17	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	17	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	19	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	19	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	23	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	23	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	25	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	25	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB2	26	0.16
(2,53)	1:9:A:ASN:HD22	1:9:A:ASN:HB3	26	0.16
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	3	0.16
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.16
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.16
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.16
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	10	0.16
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	14	0.16
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	24	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	2	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	4	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	7	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	8	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	12	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	18	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	23	0.16
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	25	0.16
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	16	0.16
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	14	0.16
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	14	0.15
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	29	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	3	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	7	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	8	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	9	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	11	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	16	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	20	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	23	0.15
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	27	0.15
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	16	0.15
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	27	0.15
(2,79)	1:2:A:VAL:H	1:3:A:HIS:H	9	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	4	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	8	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	12	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	18	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	21	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	23	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	25	0.15
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	26	0.15
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	11	0.15
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	20	0.15
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	2	0.15
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	2	0.15
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	10	0.15
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	23	0.15
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	29	0.15
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	6	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	5	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	6	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	13	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	15	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	19	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	28	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	29	0.14
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	30	0.14
(2,83)	1:6:A:ARG:H	1:7:A:GLY:H	13	0.14
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	24	0.14
(2,41)	1:8:A:ILE:H	1:8:A:ILE:HG12	22	0.14
(2,41)	1:8:A:ILE:H	1:8:A:ILE:HG13	22	0.14
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	3	0.14
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	9	0.14
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	14	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	1	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	3	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	4	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	8	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	9	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	12	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	17	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	18	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	20	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	21	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	23	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	24	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	25	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	26	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	28	0.14
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	29	0.14
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	7	0.14
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	20	0.14
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	16	0.14
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	1	0.13
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	12	0.13
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	15	0.13
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	25	0.13
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	26	0.13
(2,113)	1:2:A:VAL:HB	1:3:A:HIS:H	13	0.13
(2,106)	1:14:A:SER:H	1:13:A:SER:HA	17	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	3	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	4	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	5	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	14	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	21	0.13
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	28	0.13
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	29	0.13
(2,59)	1:13:A:SER:H	1:13:A:SER:HB3	16	0.13
(2,59)	1:13:A:SER:H	1:13:A:SER:HB2	16	0.13
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	12	0.13
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	12	0.13
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	18	0.13
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	18	0.13
(2,17)	1:2:A:VAL:H	1:2:A:VAL:HB	23	0.13
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	1	0.13
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	2	0.13
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	9	0.13
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	11	0.13
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	22	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	5	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	7	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	13	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	15	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	16	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	19	0.13
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	29	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	6	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	7	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	10	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	14	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	15	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	19	0.13
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	27	0.13
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	19	0.13
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	23	0.13
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	9	0.13
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	11	0.13
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	21	0.13
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	28	0.13
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	17	0.12
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	12	0.12
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	22	0.12
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	10	0.12
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	24	0.12
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	26	0.12
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	29	0.12
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	6	0.12
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	13	0.12
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	16	0.12
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	23	0.12
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	29	0.12
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	14	0.12
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	22	0.12
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	24	0.12
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	7	0.12
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	11	0.12
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	20	0.12
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	22	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	6	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	15	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	15	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	27	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	27	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	28	0.12
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	28	0.12
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	19	0.12
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	19	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	4	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	5	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	6	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	7	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	8	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	10	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	14	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	18	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	19	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	21	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	23	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	24	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	25	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	26	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	28	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	29	0.12
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	30	0.12
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	6	0.12
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	27	0.12
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	28	0.12
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	30	0.12
(2,12)	1:13:A:SER:H	1:13:A:SER:HA	22	0.12
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	11	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	1	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	12	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	15	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	17	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	25	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	26	0.12
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	29	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	3	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	4	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	5	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	18	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	21	0.12
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	28	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	3	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	4	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	5	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	6	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	7	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	10	0.12
(2,1)	1:2:A:VAL:H	1:2:A:VAL:HA	13	0.12
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	6	0.11
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	29	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	1	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	2	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	4	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	13	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	17	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	18	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	19	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	21	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	25	0.11
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	30	0.11
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	13	0.11
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	18	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	4	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	5	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	7	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	8	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	12	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	14	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	15	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	16	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	17	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	20	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	21	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	26	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	28	0.11
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	30	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	1	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	2	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	7	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	12	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	15	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	17	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	18	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	19	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	20	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	24	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	25	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	26	0.11
(2,95)	1:3:A:HIS:H	1:2:A:VAL:HA	27	0.11
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	7	0.11
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	20	0.11
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	23	0.11
(2,83)	1:6:A:ARG:H	1:7:A:GLY:H	15	0.11
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	2	0.11
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	9	0.11
(2,81)	1:4:A:THR:H	1:5:A:PHE:H	10	0.11
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	6	0.11
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	13	0.11
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	21	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	5	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	5	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	7	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	7	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	19	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	19	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	21	0.11
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	21	0.11
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG2	1	0.11
(2,30)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.11
(2,16)	1:17:A:LEU:H	1:17:A:LEU:HA	3	0.11
(2,15)	1:16:A:SER:H	1:16:A:SER:HA	17	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	7	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	14	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	20	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	22	0.11
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	23	0.11
(2,5)	1:6:A:ARG:H	1:6:A:ARG:HA	13	0.11
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	14	0.11
(2,4)	1:5:A:PHE:H	1:5:A:PHE:HA	18	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	1	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	8	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	12	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	13	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	15	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	16	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	17	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	25	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	26	0.11
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	29	0.11
(2,119)	1:5:A:PHE:H	1:3:A:HIS:HA	13	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	3	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	5	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	7	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	8	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	9	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	15	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	16	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	20	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	23	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	27	0.1
(2,107)	1:15:A:SER:H	1:14:A:SER:HA	29	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	1	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	3	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	4	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	5	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	6	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	7	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	8	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	9	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	14	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	15	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	17	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	20	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	21	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	23	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	25	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	27	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	28	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	29	0.1
(2,102)	1:10:A:GLY:H	1:9:A:ASN:HA	30	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	1	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	3	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	10	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	18	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	19	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	22	0.1
(2,97)	1:5:A:PHE:H	1:4:A:THR:HA	25	0.1
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	5	0.1
(2,85)	1:8:A:ILE:H	1:9:A:ASN:H	13	0.1
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	5	0.1
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	12	0.1
(2,80)	1:3:A:HIS:H	1:4:A:THR:H	28	0.1
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	1	0.1
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	1	0.1
(2,62)	1:14:A:SER:H	1:14:A:SER:HB3	29	0.1
(2,62)	1:14:A:SER:H	1:14:A:SER:HB2	29	0.1
(2,11)	1:12:A:ASN:H	1:12:A:ASN:HA	26	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	2	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	4	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	5	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	13	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	24	0.1
(2,7)	1:8:A:ILE:H	1:8:A:ILE:HA	28	0.1
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	19	0.1
(2,3)	1:4:A:THR:H	1:4:A:THR:HA	24	0.1

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

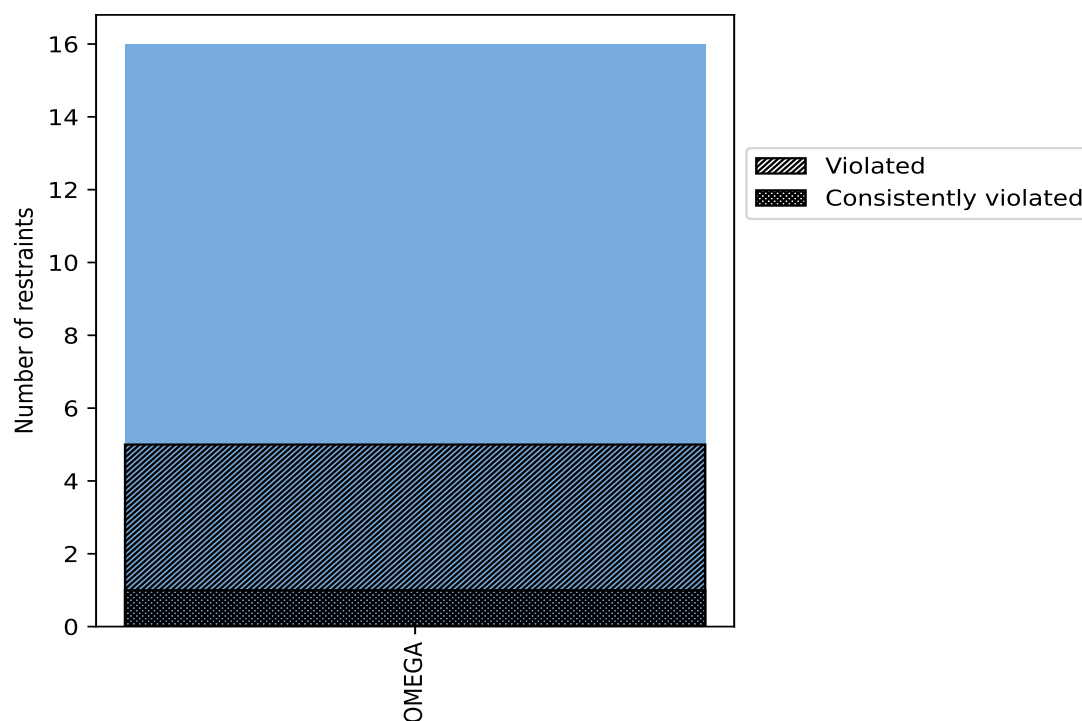
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
OMEGA	16	100.0	5	31.2	31.2	1	6.2	6.2
Total	16	100.0	5	31.2	31.2	1	6.2	6.2

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

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



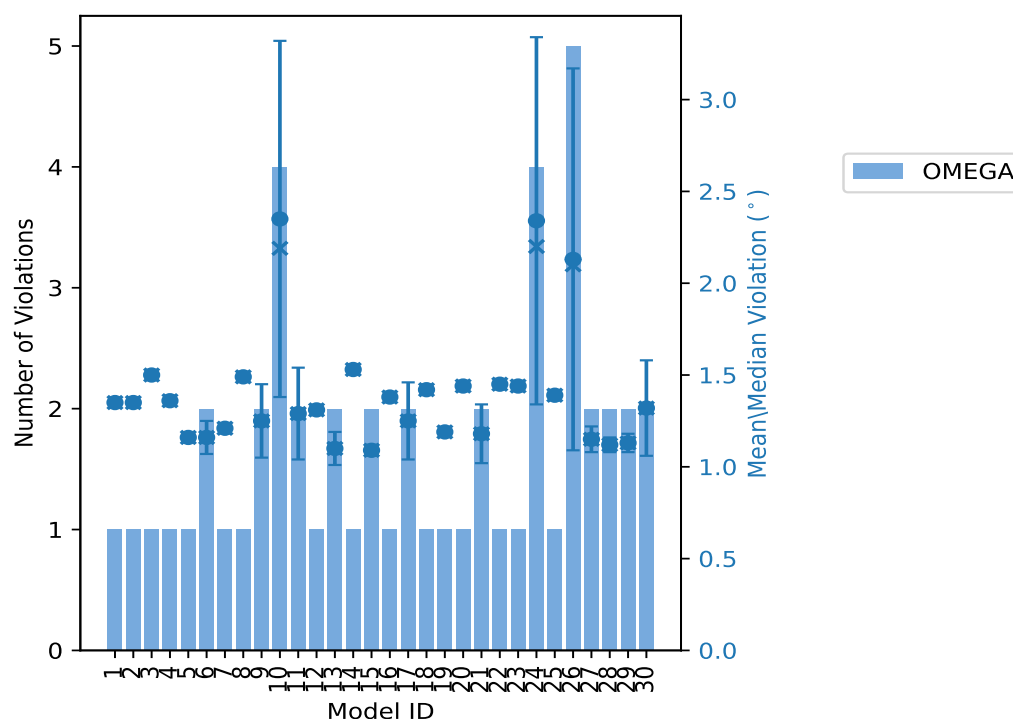
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations		Mean (°)	Max (°)	SD (°)	Median (°)
	OMEGA	Total				
1	1	1	1.35	1.35	0.0	1.35
2	1	1	1.35	1.35	0.0	1.35
3	1	1	1.5	1.5	0.0	1.5
4	1	1	1.36	1.36	0.0	1.36
5	1	1	1.16	1.16	0.0	1.16
6	2	2	1.16	1.25	0.09	1.16
7	1	1	1.21	1.21	0.0	1.21
8	1	1	1.49	1.49	0.0	1.49
9	2	2	1.25	1.45	0.2	1.25
10	4	4	2.35	3.87	0.97	2.19
11	2	2	1.29	1.54	0.25	1.29
12	1	1	1.31	1.31	0.0	1.31
13	2	2	1.1	1.19	0.09	1.1
14	1	1	1.53	1.53	0.0	1.53
15	2	2	1.09	1.12	0.03	1.09
16	1	1	1.38	1.38	0.0	1.38
17	2	2	1.25	1.46	0.21	1.25
18	1	1	1.42	1.42	0.0	1.42
19	1	1	1.19	1.19	0.0	1.19
20	1	1	1.44	1.44	0.0	1.44
21	2	2	1.18	1.34	0.16	1.18
22	1	1	1.45	1.45	0.0	1.45
23	1	1	1.44	1.44	0.0	1.44
24	4	4	2.34	3.87	1.0	2.2
25	1	1	1.39	1.39	0.0	1.39
26	5	5	2.13	4.0	1.04	2.1
27	2	2	1.15	1.22	0.07	1.15
28	2	2	1.12	1.16	0.04	1.12
29	2	2	1.13	1.18	0.05	1.13
30	2	2	1.32	1.58	0.26	1.32

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



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

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

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

Number of violated restraints		Fraction of the ensemble	
OMEGA	Total	Count ¹	%
1	1	1	3.3
0	0	2	6.7
2	2	3	10.0
0	0	4	13.3
0	0	5	16.7
0	0	6	20.0
0	0	7	23.3
0	0	8	26.7
0	0	9	30.0
0	0	10	33.3
0	0	11	36.7

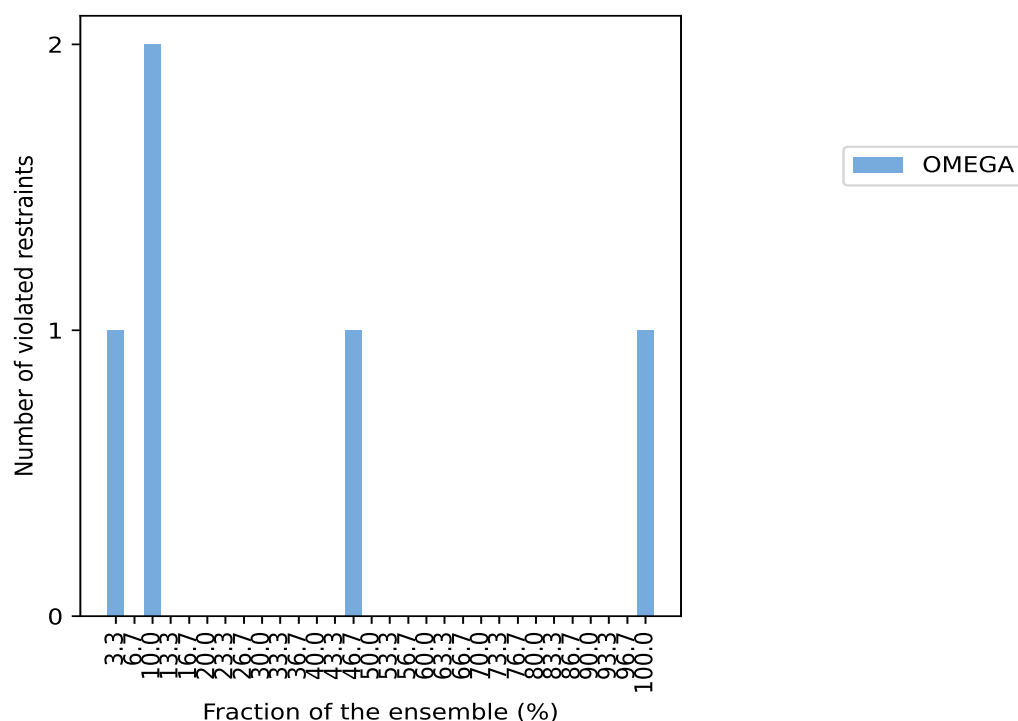
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Number of violated restraints		Fraction of the ensemble	
OMEGA	Total	Count ¹	%
0	0	12	40.0
0	0	13	43.3
1	1	14	46.7
0	0	15	50.0
0	0	16	53.3
0	0	17	56.7
0	0	18	60.0
0	0	19	63.3
0	0	20	66.7
0	0	21	70.0
0	0	22	73.3
0	0	23	76.7
0	0	24	80.0
0	0	25	83.3
0	0	26	86.7
0	0	27	90.0
0	0	28	93.3
0	0	29	96.7
1	1	30	100.0

¹ Number of models with violations

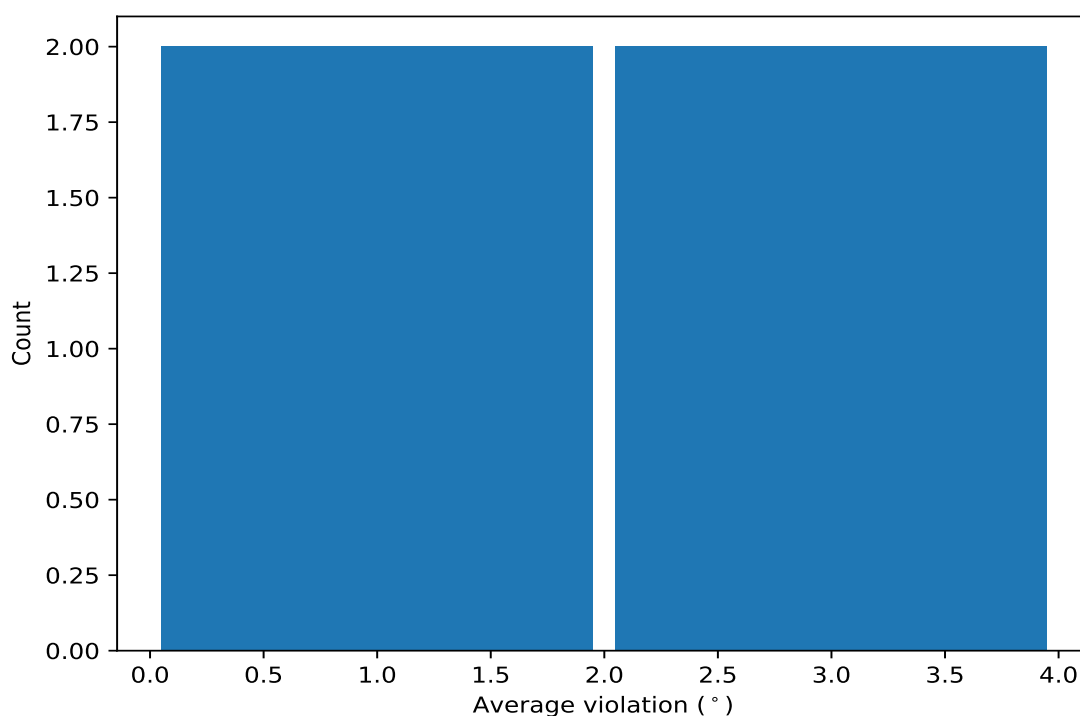
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

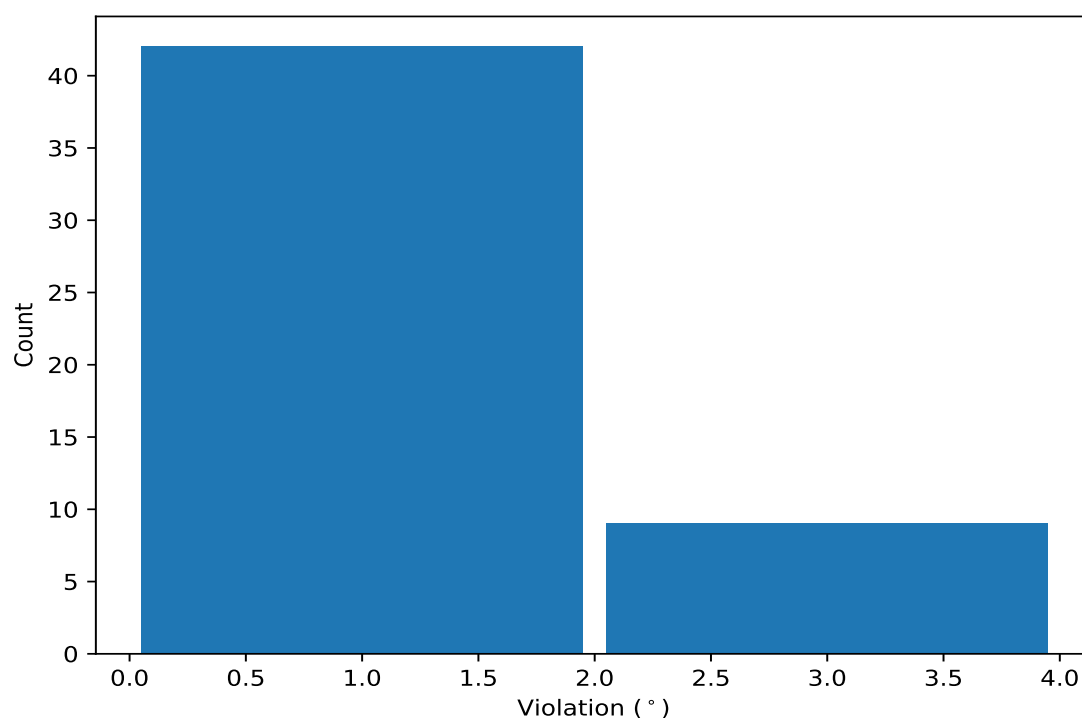
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	30	1.44	0.29	1.38
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	14	1.07	0.04	1.06
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:SER:N	1:13:A:SER:CA	3	3.91	0.06	3.87
(1,11)	1:11:A:HIS:CA	1:11:A:HIS:C	1:12:A:ASN:N	1:12:A:ASN:CA	3	2.14	0.06	2.1

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:SER:N	1:13:A:SER:CA	26	4.0
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:SER:N	1:13:A:SER:CA	10	3.87
(1,12)	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:SER:N	1:13:A:SER:CA	24	3.87
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	10	2.29
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	24	2.29
(1,11)	1:11:A:HIS:CA	1:11:A:HIS:C	1:12:A:ASN:N	1:12:A:ASN:CA	26	2.22
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	26	2.1
(1,11)	1:11:A:HIS:CA	1:11:A:HIS:C	1:12:A:ASN:N	1:12:A:ASN:CA	24	2.1
(1,11)	1:11:A:HIS:CA	1:11:A:HIS:C	1:12:A:ASN:N	1:12:A:ASN:CA	10	2.09
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	30	1.58
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	11	1.54
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	14	1.53
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	3	1.5
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	8	1.49
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	17	1.46
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	9	1.45
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	22	1.45
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	20	1.44
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	23	1.44
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	18	1.42
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	25	1.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	16	1.38
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	4	1.36
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	1	1.35
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	2	1.35
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	21	1.34
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	12	1.31
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	6	1.25
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	27	1.22
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	7	1.21
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	13	1.19
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	19	1.19
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	29	1.18
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	5	1.16
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	28	1.16
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	10	1.16
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	26	1.16
(1,13)	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	1:14:A:SER:CA	26	1.15
(1,14)	1:14:A:SER:CA	1:14:A:SER:C	1:15:A:SER:N	1:15:A:SER:CA	15	1.12
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	24	1.08
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	27	1.08
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	29	1.08
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	28	1.07
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	6	1.06
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	15	1.06
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	30	1.06
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	9	1.05
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	11	1.04
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	17	1.04
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	21	1.02
(1,10)	1:10:A:GLY:CA	1:10:A:GLY:C	1:11:A:HIS:N	1:11:A:HIS:CA	13	1.01